

### Compute Motor Vehicle Emissions Estimates

The mobile source emission processor computes day-specific, gridded, hourly motor vehicle emissions estimates of VOC total organic gases (TOG), carbon monoxide (CO), and oxides of nitrogen (NO<sub>x</sub>). The actual emission estimate computations performed and maintained in the MEPPS data base are as follows:

- TOG for gasoline (noncatalyst/catalyst composite) evaporative diurnal processes;
- TOG for gasoline (noncatalyst/catalyst composite) evaporative nondiurnal processes;
- TOG for gasoline (noncatalyst/catalyst composite) exhaust operations;
- NO<sub>x</sub> for gasoline (noncatalyst/catalyst composite) exhaust operations;
- CO for gasoline (noncatalyst/catalyst composite) exhaust operations;
- TOG for diesel (noncatalyst/catalyst composite) exhaust operations;
- NO<sub>x</sub> for diesel (noncatalyst/catalyst composite) exhaust operations; and
- CO for diesel (noncatalyst/catalyst composite) exhaust operations.

The mobile emission processor computes motor vehicle emissions estimates based on three types of VMT files:

- On-network VMT;
- Off-network VMT; and
- Public land survey quarter sections VMT.

The differences in the VMT types are:

- On-network VMT are network link-specific;
- Off-network VMT are county/area type/facility type-specific; and
- Public land survey quarter sections VMT are county/polygon/area type/facility type-specific.

The mobile-emission processor estimates motor vehicle emissions for all combinations of VMT. Regardless of the VMT type that is used to generate motor vehicle emission estimates, all motor-vehicle emission estimates have some degree of uncertainty. However, the most desirable motor-vehicle emissions estimates usually are generated from on-network, link-specific data, followed by public land survey quarter sections data, and finally off-network data. Motor vehicle emission estimates that are generated from on-network data are not more certain, but that they are more spatially representative.

Before the mobile-source emission processor computes the motor vehicle emission estimates, it computes a fleet composite emission factor. Equations 4-44 through 4-67 show how the processor computes the fleet composite emission factors. In all cases, the emission factors are extracted from the Mobile lookup tables based on the appropriate indices. Please refer to the

section on generating the Mobile emission factors lookup tables earlier in this section for additional information.

If the user has provided non-I/M-specific VMT, the mobile source emission processor computes the fleet composite emission factors by vehicle classification for temperature and speeds combinations through the application of Equations 4-35 through 4-42.

$$hcdif_{s,t} = \sum_j hcdi_{j,s,t} * vmix_j \quad (4-35)$$

$$hcexf_{s,t} = \sum_j hcex_{j,s,t} * vmix_j \quad (4-36)$$

$$nox_{s,t} = \sum_j noxx_{j,s,t} * vmix_j \quad (4-37)$$

$$coex_{s,t} = \sum_j coex_{j,s,t} * vmix_j \quad (4-38)$$

$$hcevf_{s,t} = \sum_j hcev_{j,s,t} * vmix_j \quad (4-39)$$

$$dhcex_{s,t} = \sum_j dhcex_{j,s,t} * vmix_j \quad (4-40)$$

$$dnox_{s,t} = \sum_j dnoxx_{j,s,t} * vmix_j \quad (4-41)$$

$$dcoex_{s,t} = \sum_j dcoex_{j,s,t} * vmix_j \quad (4-42)$$

where:  $j$  is the vehicle classification index

$s$  is the speed index

$t$  is the temperature index

$hcdif$  is the hydrocarbon diurnal fleet composite emission factor for all vehicle types (grams/mile)

$hcdi$  is the non-I/M hydrocarbon diurnal emission factor (grams/mile)

$vmix$  is the vehicle mix profile

$hcexf$  is the hydrocarbon exhaust nondiurnal fleet composite emission factor for gasoline vehicles (grams/mile)

$hcex$  is the non-I/M hydrocarbon exhaust nondiurnal emission factor for gasoline vehicles (grams/mile)

$nox_{s,t}$  is the oxides of nitrogen exhaust nondiurnal fleet composite emission factor for gasoline vehicles (grams/mile)

$noxx$  is the non-I/M oxides of nitrogen exhaust nondiurnal emission factor for gasoline vehicles (grams/mile)

$coex_{s,t}$  is the carbon monoxide exhaust nondiurnal fleet composite emission factor for gasoline vehicles (grams/mile)

$coex$  is the non-I/M carbon monoxide exhaust nondiurnal emission factor for gasoline vehicles (grams/mile)

$hcevf_{s,t}$  is the hydrocarbon evaporative nondiurnal fleet composite emission factor for gasoline vehicles (grams/mile)

$hcev$  is the non-I/M hydrocarbon evaporative nondiurnal emission factor for gasoline vehicles (grams/mile)

$dhcex_{s,t}$  is the hydrocarbon exhaust nondiurnal fleet composite emission factor for diesel vehicles (grams/mile)

$dhcex$  is the non-I/M hydrocarbon exhaust nondiurnal emission factor for diesel vehicles (grams/mile)

dnox<sub>f</sub> is the oxides of nitrogen exhaust nondiurnal fleet composite emission factor for diesel vehicles (grams/mile)

dnox<sub>x</sub> is the non-I/M oxides of nitrogen exhaust nondiurnal emission factor for diesel vehicles (grams/mile)

dcoex<sub>f</sub> is the carbon monoxide exhaust nondiurnal fleet composite emission factor for diesel vehicles (grams/mile)

dcoex<sub>x</sub> is the non-I/M carbon monoxide exhaust nondiurnal emission factor for diesel vehicles (grams/mile)

If the user has provided I/M-specific VMT data, the processor computes the fleet composite emission factors by vehicle category for temperature and speed combinations through the application of Equations 4-43 through 4-50.

$$hcdif_{s,t} = \sum_j ihcdi_{j,s,t} * vmix_j \quad (4-43)$$

$$hcexf_{s,t} = \sum_j ihcex_{j,s,t} * vmix_j \quad (4-44)$$

$$nox_{f,s,t} = \sum_j inoxx_{j,s,t} * vmix_j \quad (4-45)$$

$$coexf_{s,t} = \sum_j icoex_{j,s,t} * vmix_j \quad (4-46)$$

$$hcevf_{s,t} = \sum_j ihcev_{j,s,t} * vmix_j \quad (4-47)$$

$$dhcexf_{s,t} = \sum_j idhcex_{j,s,t} * vmix_j \quad (4-48)$$

$$dnox_{f,s,t} = \sum_j idnox_{j,s,t} * vmix_j \quad (4-49)$$

$$dcoexf_{s,t} = \sum_j idcoex_{j,s,t} * vmix_j \quad (4-50)$$

where:

- ihcdi is the I/M hydrocarbon diurnal emission factor (grams/mile)
- ihcex is the I/M hydrocarbon exhaust nondiurnal emission factor for gasoline vehicles (grams/mile)
- inoxx is the I/M oxides of nitrogen exhaust nondiurnal emission factor for gasoline vehicles (grams/mile)
- icoex is the I/M carbon monoxide exhaust nondiurnal emission factor for gasoline vehicles (grams/mile)
- ihcev is the I/M hydrocarbon evaporative nondiurnal emission factor for gasoline vehicles (grams/mile)
- idhcex is the I/M hydrocarbon exhaust nondiurnal emission factor for diesel vehicles (grams/mile)
- idnox<sub>x</sub> is the I/M oxides of nitrogen exhaust nondiurnal emission factor for diesel vehicles (grams/mile)
- idcoex is the I/M carbon monoxide exhaust nondiurnal emission factor for diesel vehicles (grams/mile)

If the user has provided both I/M and non-I/M VMT data, the mobile source emission processor computes the fleet composite emission factors by vehicle category for temperature and speed combinations through the application of Equations 4-51 through 4-58. This set of equations can be applied only to on-network VMT data because the I/M percentages are input to the mobile source emission processor on a link-specific basis.

$$hcdif_{s,t} = \sum_j ((ihcdi_{j,s,t} * imvmt_l) + (hcdi_{j,s,t} * (1 - imvmt_l))) * vmix_j \quad (4-51)$$

$$hcexf_{s,t} = \sum_j ((ihcex_{j,s,t} * imvmt_l) + (hcex_{j,s,t} * (1 - imvmt_l))) * vmix_j \quad (4-52)$$

$$nox_{s,t} = \sum_j ((inoxx_{j,s,t} * imvmt_l) + (noxx_{j,s,t} * (1 - imvmt_l))) * vmix_j \quad (4-53)$$

$$coexf_{s,t} = \sum_j ((icoex_{j,s,t} * imvmt_l) + (coex_{j,s,t} * (1 - imvmt_l))) * vmix_j \quad (4-54)$$

$$hcevf_{s,t} = \sum_j ((ihcev_{j,s,t} * imvmt_l) + (hcev_{j,s,t} * (1 - imvmt_l))) * vmix_j \quad (4-55)$$

$$dhcexf_{s,t} = \sum_j ((idhcex_{j,s,t} * imvmt_l) + (dhcex_{j,s,t} * (1 - imvmt_l))) * vmix_j \quad (4-56)$$

$$dnox_{s,t} = \sum_j ((idnox_{j,s,t} * imvmt_l) + (dnnox_{j,s,t} * (1 - imvmt_l))) * vmix_j \quad (4-57)$$

$$dcoexf_{s,t} = \sum_j ((idcoex_{j,s,t} * imvmt_l) + (dcoex_{j,s,t} * (1 - imvmt_l))) * vmix_j \quad (4-58)$$

where:  $imvmt$  is the fraction of vehicles that are under an I/M program; and  
 $l$  is the link identifier index.

Many indices have been left out of Equations 4-35 through 4-58. The composite emission factors that are generated are gridded, hourly values. Because temperature is a gridded, hourly value, the temperature index  $t$  in Equations 4-31 through 4-54 implies that the composite emissions factor are gridded, hourly values.

Once the fleet composite emission factors have been computed, the mobile source emission processor computes the motor vehicle emission estimates through the application of Equations 4-59 through 4-66.

$$dhc\_vee = hcdif * divmt * 10^{-3} \quad (4-59)$$

$$hc\_xee = hcexf * ovmt * 10^{-3} \quad (4-60)$$

$$nox\_xee = noxf * ovmt * 10^{-3} \quad (4-61)$$

$$co\_xee = coexf * ovmt * 10^{-3} \quad (4-62)$$

$$hc\_vee = hcevf * ovmt * 10^{-3} \quad (4-63)$$

$$dhc\_xee = dhcexf * ovmt * 10^{-3} \quad (4-64)$$

$$dnox\_xee = dnnox * ovmt * 10^{-3} \quad (4-65)$$

$$dco\_xee = dcof * ovmt * 10^{-3} \quad (4-66)$$

where:  $dhc\_vee$  is the gridded, hourly diurnal hydrocarbon emission estimate (kilograms)  
 $divmt$  is the gridded, hourly diurnal VMT (miles)  
 $hc\_xee$  is the gridded, hourly exhaust hydrocarbon nondiurnal emission estimate for gasoline vehicles (kilograms)  
 $ovmt$  is the gridded, hourly nondiurnal VMT (miles)  
 $nox\_xee$  is the gridded, hourly exhaust oxides of nitrogen nondiurnal emission estimate for gasoline vehicles (kilograms)  
 $co\_xee$  is the gridded, hourly exhaust carbon monoxide nondiurnal emission estimate for gasoline vehicles (kilograms)  
 $hc\_vee$  is the gridded, hourly evaporative hydrocarbon nondiurnal emission estimate for gasoline vehicles (kilograms)

dhc\_xee is the gridded, hourly exhaust hydrocarbon nondiurnal emission estimate for diesel vehicles (kilograms)  
 dnoxxee is the gridded, hourly exhaust oxides of nitrogen nondiurnal emission estimate for diesel vehicles (kilograms)  
 dco\_xee is (the gridded, hourly exhaust carbon monoxide nondiurnal emission estimate for diesel vehicles (kilograms)

The mobile-source emission processor computes the final motor vehicle emission estimates file by summing the emission estimates computed by Equations 4-59 through 4-66 over each state identifier, county identifier, east-west grid cell identifier, north-south grid cell identifier, process type (EV for evaporative, EX for exhaust), technology type (1 for gasoline, 2 for diesel), and pollutant identifier (HC for hydrocarbon, CO for carbon monoxide, NO<sub>x</sub> for oxides of nitrogen).

### The PART5 Model

The current version of PART5 was released in 1995 by the U.S. EPA Office of Mobile Sources. The description given here is taken principally from the user's guide, *A Draft User's Guide to PART5: A Program for Calculating Particle Emissions from Motor Vehicles* (U.S. EPA, 1995b), which provides information in addition to that given in this section. The guide is available from the Office of Mobile Sources Internet web site at <http://www.epa.gov/omsw/models.htm>. The PART5 is a FORTRAN program used to model emission factors needed to estimate emissions from gasoline and diesel powered on-road vehicles. It calculates particle emission factors in grams per mile for particle sizes 1 to 10 micrometers. The emission factors include exhaust particulate matter and components, brake wear, tire wear, and re-entrained road dust. The program includes default data for most inputs, but allows user-supplied data for most items. The interactive aspects of running PART5, as it is provided by the Office of Mobile Sources, have been subsumed into MEPPS to allow the user to enter and edit data, specify program control flags, and run the model via a series of windows within the EMPRO mobile source processor.

Controls specified within PART5 may vary spatially and temporally. PART5 output report flags are not germane within MEPPS because the outputs are automatically processed with emissions from other emission sources in MEPPS internal format. The flags used include the following items:

- Vehicle fleet mix. The user may specify of whether default or user-supplied VMT vehicle fleet mixes are used. The VMT mix is the fraction of total VMT for all vehicles contributed to by each vehicle class. The default VMT is based on national averages and trends over the years. The trends reflect the sales shift from automobiles to light-duty trucks, and the increasing use of diesel engines in both light and heavy-duty trucks. VMT mix may vary spatially. The following are the descriptions of the vehicle classes and corresponding Federal Highway Administration (FHA) and gross vehicle weight (GVW) used in PART5.

Vehicle Class	FHA Class	GVW (lbs)
1 = LDGV (light-duty gasoline vehicle)		
2 = LDGT1 (light-duty gasoline truck, I)	1	<6000
3 = LDGT2 (light-duty gasoline truck II)	2A	6001-8500
4 = HDGV (heavy-duty gasoline truck)	2B-8B	>8500
5 = MC (motor cycle)		
6 = LDDV (light-duty diesel vehicle)	1	<6000
7 = LDDT (light-duty diesel truck)	2A	6001-8500
8 = 2BHDDV (class 2B heavy duty diesel vehicle)	2B	8501-10000
9 = LHDDV (light heavy-duty diesel vehicle)	3,4,5	10001-19500
10 = MHDDV (medium heavy-duty diesel vehicle)	6,7,8A	19501-33000
11 = HHDDV (heavy heavy-duty diesel vehicle)	8B	33000+
12 = BUSES (buses)		

- Mileage accumulation rates. The user may supply or use default mileage accumulation rates and vehicle registration distributions. The mileage accumulation rate is the expected number of miles that a typical vehicle (for each class) is expected to travel in a year, divided by 100,000. The rates must be provided for each vehicle type for each of 25 years (12 years for motor cycles).
- Inspection and maintenance. The user specifies whether an inspection and maintenance program is assumed for gasoline vehicle vehicles only.
- Reformulated gasoline. The specifies whether the use and effects of reformulated gasoline on particulate emissions are assumed. The effects are partially based on the sulfur content of gasoline used. An average sulfur weight percent of 0.034 is used for any gasoline used in all years prior to 2000. If reformulated gasoline is used for the year 2000 or later, the sulfur weight percent is assumed to be 0.0138.

The purpose of MEPPS is to estimate temporally and spatially-varying emission data on a gridded basis. This is consistent with some additional input data which PART5 requires be entered on spatial basis, which are defined as PART5 scenarios. In EMPRO mobile source processing the user is prompted to edit existing or new scenario data. The information includes:

- Region, calendar year, speed cycle (type of driving, ie. cruise), and average speed.
- Percent of unpaved road silt, paved road silt loading in gm /m<sup>2</sup>, and optionally, the average number of wheels per vehicle. Modeled dust emission factor are highly sensitive to the unpaved road silt percentage which is extremely variable. Consequently, measured data are advised when possible.

- The number of days each year with greater than 0.01 inches of precipitation for use in modeling re-entrained dust. This is climatological average data. In the future, the emission processing system may be modified to use more spatially and temporally accurate modeled precipitation data by grid cell taken from MM5 and MCIP for the PART5 calculations.
- A scenario name may be applied. In MEPPS a FIPS code a geographic identifier is entered which is used to apply PART5 emission factors computed for the county level to the appropriate modeling grid cells.
- PART5 expects the user to define a maximum particle size cutoff (maximum allowed is 10 micrometers). In MEPPS the maximum size is defaulted to 10 micrometers to ensure that the full range of particle sizes are represented in the regional emission estimates.
- Average vehicle weight (lbs)

### PART5 Emission Factors

The emission factors calculated by PART5 include the particulate pollutant compounds of lead, sulfate, soluble organic fraction particulate matter, remaining carbon portion particulate matter, and total exhausted particulate. The lead and sulfate are formed from the lead and sulfur contained in the fuel. The soluble organic fraction consists primarily of hydrocarbons coming from unburned or partially burned fuel and lubricating oil. The remaining carbon portion consists of soot-like carbon (elemental carbon) and trace amounts of other components from the fuel and lubricating oil. The total exhaust particulate is the sum of these four categories. In addition to these categories of exhaust emissions, idle exhaust emissions (for heavy diesel vehicles only), brake wear, tire wear, fugitive dust, indirect sulfate, and gaseous sulfur dioxide are calculated by PART5.

The model calculates the emission factors for the 12 vehicle classes previously described and a fleet-wide average (estimated by VMT weighting of the emission factors for each of the 12 vehicle classes). The factors are composites of the emission factors for the 25+ years prior to the year of interest, in order to allow for the effects of older vehicles. The composite emission factor for each vehicle class is calculated by weighting the emission factor calculated for each model year by the travel fraction for that model year, and then summing the 25 weighted factors. The travel fraction of a model year is the fraction of VMT by a vehicle of that model year out of the total number of miles traveled by all model years' vehicles in that vehicle class.

$$EFCOMP_v = \sum_{m=1}^{25} EF_{m,v} * TF_{m,v} \quad (4-67)$$

where:  $EFCOMP_v$  is the composite emission factor for vehicle class  $v$ ,

EF<sub>m,v</sub> is the emission factor for vehicle class v, model year m,  
 TF<sub>m,v</sub> is the travel fraction for vehicle class v, model year m.

The overall travel fraction of a vehicle class represents the fraction of the total number of VMT of that class of the total highway VMT by all 12 classes. The VMT fractions for each vehicle class are multiplied by the corresponding composite emission factors (EFCOMP<sub>v</sub>), and the sum of the adjusted emission factors is reported as the emission factor for all vehicles.

$$EF_{ALL} = \sum EFCOMP_v * TFCLASS_v \quad (4-68)$$

where: EF<sub>ALL</sub> is the weighted emission factor for all vehicles,  
 TFCLASS<sub>v</sub> is the VMT of vehicle class v.

The emission factor for all vehicles, EF<sub>ALL</sub>, represents the grams/mile of emissions

#### Lead Emission Factors for gasoline-fueled vehicles

Lead particulate emission factors for gasoline-fueled vehicles assume that almost all lead in the fuel is exhausted. Therefore, the emission factors (grams/mile) depend on the lead content of fuel and fuel economy of the vehicle (miles/gallon). The factors allow for the fact that the lead content of leaded fuel is much greater than for unleaded fuel. *The assumption is made that because diesel fuel has negligible lead content, the lead emissions from diesel vehicles will be negligible.* The following formulae are used to compute lead emission factors for all gasoline-fueled automobiles and motorcycles, respectively.

$$LEAD_{m,v} = PLNOCT_{m,v} * VLNOCT_{m,v} + PUNOCT_{m,v} * VUNOCT_{m,v} + \\
 PLYSCT_{m,v} * VLYSCT_{m,v} + PUYSCT_{m,v} * VUYSCT_{m,v} \quad (4-69)$$

where: m denotes a specified model year  
 v denotes a specified vehicle class  
 LEAD<sub>m,v</sub> is the lead particulate emissions for any given vehicle (grams/mile)  
 PLNOCT<sub>m,v</sub> is the emissions for a non-catalyst, leaded fuel vehicle (grams/mile)  
 PUNOCT<sub>m,v</sub> is the emissions for a non-catalyst, unleaded fuel vehicle (grams/mile)  
 PLYSCT<sub>m,v</sub> is the emissions for a catalyst, leaded fuel vehicle (grams/mile)  
 PUYSCT<sub>m,v</sub> is the emissions for a catalyst, unleaded fuel vehicle (grams/mile)  
 VLNOCT<sub>m,v</sub> is the emissions for a non-catalyst, leaded fuel vehicle (grams/mile)  
 VUNOCT<sub>m,v</sub> is the emissions for a non-catalyst, unleaded fuel vehicle (grams/mile)  
 VLYSCT<sub>m,v</sub> is the fraction of catalyst leaded fuel vehicles  
 VUYSCT<sub>m,v</sub> is the fraction of catalyst, unleaded fuel vehicles

The emission rate is adjusted for speed by the factor FEC such that:

$$CLEAD_{m,v} = FEC * LEAD_{m,v} \quad (4-70)$$



where:  $CLEAD_{m,v}$  is the lead emissions for a vehicle of model year  $m$  and vehicle class  $v$ , which has been adjusted for the effect of speed (grams/mile)

$$FEC \text{ is } 1/SCF_c \quad (4-71)$$

$SCF_c$  is the speed correction factor, based either transient driving cycle ( $c=1$ ) or steady cruise driving cycle ( $c=2$ )

$$SCF_1 = 0.17930 + (0.038561 * SPEED_v) - (0.00041067 * SPEED_v^2) \quad (4-72)$$

$$SCF_2 = 0.26929 + (0.054607 * SPEED_v) - (0.00069818 * SPEED_v^2) \quad (4-73)$$

$SPEED_v$  is the average speed for vehicle class  $v$  (mph) - user input

Motorcycles do not have catalytic emission controls, therefore organic emission factors are not calculated and sulfate emission factors are deemed negligible. PART5 emission factors for motorcycles are almost entirely for lead particulate matter. The lead particulate emission factor for 2-stroke engines is 0.33 g/mi and for 4-stroke engines 0.046 grams/mile. For model years before 1978 there were 51 percent 4-stroke engines and 49 percent 2-stroke engines, computed as follows:

$$LEAD_{m, motorcycle} = [(0.49 * 0.33) + (0.51 * 0.046)] * PSL \quad (4-74)$$

For model years 1978 and later motorcycles are assumed to consist entirely of 4-stroke engines:

$$LEAD_{m, motorcycle} = 0.046 * PSL \quad (4-75)$$

where:  $PSL$  is the fraction of all particles that are emitted based on a specified upper particle size cutoff (10 micrometers running in MEPPS)

The specific derivations of the lead particulate emission formulae are given in Appendix 1 of the PART 5 user's guide (U.S. EPA, 1995b).

#### Sulfate Emission Factors for Gasoline-Fueled Vehicles

Particulate sulfate emission factors consist of direct and indirect sulfate material. The direct sulfate is exhausted as sulfuric acid, and the indirect sulfate is formed later in the atmosphere from exhausted  $SO_2$ . The indirect sulfate in the model is calculated based on the assumption that it consists entirely of ammonium sulfate and ammonium bisulfate. The direct sulfate, indirect sulfate, and gaseous sulfate emission factors are computed in PART5, and the emission factors reported as grams/mile traveled.

The direct sulfate from non-catalyst vehicles using leaded fuel (includes catalyst-equipped vehicles which are misfueled, making the catalyst ineffective) is calculated as:

$$DSULFN = .002, \text{ for speeds equal to or less than } 19.6 \text{ mph} \quad (4-76)$$

$$DSULFN = .001, \text{ for speeds equal to or greater than } 34.8 \text{ mph} \quad (4-77)$$

The direct sulfate from catalyst vehicles is calculated as :

$$DSULFC_{m,v} = [FRAC_{cat/no\ air} (.005) + FRAC_{cat/air} (.016)] \quad (4-78)$$

for speeds equal to or less than 19.6 mph

$$DSULFC_{m,v} = [FRAC_{ox/noair} (.005) + FRAC_{3w/noair} (.001) + FRAC_{ox/air} (.020) + FRAC_{3w/air} (.025)] \quad (4-79)$$

for speeds equal to or greater than 34.8 mph

For speeds between 19.6 and 34.8 mph, DSULFN and DSULFC are interpolated between Equations 4-76 and 4-77 and 4-78 and 4-79, respectively.

where:

- m denotes a specified model year
- v denotes a specified vehicle class
- $FRAC_{cat/noair}$  is the fraction of vehicles which are catalyst equipped with no air pump
- $FRAC_{cat/air}$  is the fraction of vehicles which are catalyst equipped with an air pump
- $FRAC_{ox/noair}$  is the fraction of vehicles which are oxygen catalyst equipped with no air pump
- $FRAC_{3w/noair}$  is the fraction of vehicles which are 3-way catalyst equipped with no air pump
- $FRAC_{ox/air}$  is the fraction of vehicles which are oxidation catalyst equipped with an air pump
- $FRAC_{3w/air}$  is the fraction of vehicles which are 3-way catalyst equipped with air pump

The direct sulfate from all gasoline-fueled vehicles is computed as:

$$DSULF_{m,v} = CTLFRC_{m,v} * DSULFC_{m,v} + (1.0 - CTLFRC_{m,v}) * DSULFN \quad (4-80)$$

where:  $CTLFRC_{m,v} = CATFCT_{m,v} (1 - RMIS_{m,v}) \quad (4-81)$   
the fraction of the vehicle class that has an effective catalyst

The PART5 assumes that all sulfur in fuel is exhausted as either sulfate or gaseous sulfur dioxide ( $SO_2$ ). Therefore when the direct sulfate emission factor is calculated, the remaining sulfur in the fuel is considered to be exhausted as  $SO_2$ . The amount of sulfur remaining in the fuel after the

direct sulfate emission factor has been determined must be calculated to find the amount of sulfur exhausted as SO<sub>2</sub> (grams/mile).

The following equation is used to determine the fraction of sulfur in the fuel that has been directly converted to sulfate (DSULF<sub>m,v</sub> calculated in Equation 4-80 above). The equation calculates direct sulfate as a function of the fuel sulfur content, DCNVRT (the fraction of sulfur in the fuel that is converted to direct sulfate), and the fuel economy.

$$\text{DSULF}_{m,v} = \frac{13.6078 * (1.0 + \text{WATER}) * \text{FDNSTY} * \text{SWGHT} * \text{DCNVRT}}{\text{FE}_{m,v}} \quad (4-82)$$

where: m denotes a given model year  
v denotes a given vehicle class  
DSULF<sub>m,v</sub> is the direct sulfate emission factor (grams/mile)  
WATER is the weight ratio of seven water molecules to sulfate, 1.2857, based the estimate that at 50 percent humidity, seven water molecules bond with each sulfuric acid molecule  
FDNSTY is the fuel density in lb/gal (6.09 pounds/gallon)  
FE<sub>m,v</sub> is the fuel economy  
SWGHT is the weight percent of sulfur content in fuel (.034, except for reformulated fuel phase II, for year 2000 and later .0138)  
DNVRT is the percent of sulfur in the fuel that is directly converted into sulfate (2 percent)  
13.6078 is a unit conversion factor equal to (453.592 \* 3.0)/100, where 453. 592 is equal to the number of gram in a pound, 3.0 is the weight ratio of sulfate to sulfur, and division by 100 corrects for the weight percent of sulfur, SWGHT

If DSULFC<sub>m,v</sub> and DSULFN (from Equations 4-76 through 4-79) are substituted in Equation 4-82, one can solve for the fractions of sulfur in the fuel that are converted to sulfate separately for catalyst and noncatalyst vehicles:

$$\text{FCNVRC}_{m,v} = \frac{\text{DSULFC}_{m,v} * \text{FE}_{m,v}}{\text{FDNSTY} * \text{SWGHT}} / (13.6078 * (1.0 + \text{WATER}) * \text{FDNSTY} * \text{SWGHT}) \quad (4-83)$$

$$\text{FCNVRN}_{m,v} = \frac{\text{DSULFN} * \text{FE}_{m,v}}{\text{FDNSTY} * \text{SWGHT}} / (13.6078 * (1.0 + \text{WATER}) * \text{FDNSTY} * \text{SWGHT}) \quad (4-84)$$

where: FCNVRC<sub>m,v</sub> is the fraction of the percent of fuel that is directly converted into sulfate for catalyst equipped vehicles  
FCNVRN<sub>m,v</sub> is the fraction of the percent of fuel that is directly converted into sulfate for non-catalyst vehicles

The gaseous sulfur emission factors, which are dependent on the above fractions, are calculated from the following equation:

$$SO2_{m,v} = 9.072 * FDNSTY * SWGHT * (1.0 - DCNVRT) / FE_{m,v} \quad (4-85)$$

where:  $SO2_{m,v}$  is the gaseous sulfur emission factor of a vehicle  
 9.072 is a unit conversion factor equal to  $(453.592 * 2) / 100$ , where 453.592 is the number of grams in a pound, 2 is the weight ratio of  $SO_2$  to sulfur, and the division by 100 corrects for the weight percent of sulfur, SWGHT

Additional details concerning the calculation of gaseous sulfur emission factors are given in the PART5 user's guide (U.S. EPA, 1995b). In addition to direct sulfate and gaseous sulfate emission factors, PART5 estimates an indirect sulfate emission factor by assuming that a fraction of the gaseous sulfur dioxide emissions is later converted in the atmosphere to sulfate material. Based on ambient sulfur and sulfate measurements in 11 cities, it is estimated that 12 percent of all gaseous sulfur is converted to sulfate. Additional information on the calculation of indirect sulfate is given in the PART5 user's guide.

#### Sulfate Emission Factors for Diesel-Fueled Vehicles

For diesel-fueled vehicles, PART5 calculates sulfate emission factors again assuming that all sulfur in the fuel is exhausted as either sulfuric acid or gaseous sulfur dioxide. The direct sulfate emission factor (grams/mile) is calculated using the following equation:

$$DSULF_{m,v} = 13.6078 * (1.0 + WATER) * FDNSTY * SWGHTD * DCNVRT / FE_{m,v} \quad (4-86)$$

where: m is a specified model year  
 y is a specified vehicle class  
 $DSULF_{m,v}$  is the direct sulfate emission factor for a vehicle (grams/mile)  
 DCNVRT is the fraction of sulfur in the fuel that is converted directly to sulfate (2.0 percent)

FDNSTY is the density of diesel fuel (7.11 pounds/gallon)

$FE_{m,v}$  is the fuel economy for a vehicle (miles/gallon)

SWGHTD is the weight percent of sulfur in diesel fuel (0.25 for high sulfur fuel, 0.05 for low sulfur fuel used in 1993 and later)

WATER is the weight ratio of seven water molecules to sulfate (1.2857)

13.6078 is a unit conversion factor equal to  $493.592 * 3 / 100$ , where 493.592 is the number of grams in a pound, 3 is the weight ratio of sulfate to sulfur, and the division by 100 corrects for the weight percent of sulfur SWGHTD

The gaseous sulfur emission factor is calculated by the following equation:

$$87) \quad \text{SO2}_{m,v} = 9.072 * \text{FDNSTY} * \text{SWGHTD} * (1.0 - \text{DCNVRT}) / \text{FE}_{m,v} \quad (\text{Eq.4-})$$

where:

$\text{SO2}_{m,v}$  is the sulfur emission factor (grams/mile) of a vehicle

9.072 is a unit conversion factor equal to  $(453.592 * 2/100)$  where 453.592 is the number of grams in a pound, 2 is the weight ratio of  $\text{SO}_2$  to sulfur, and the division by 100 corrects for the weight percent of sulfur, SWGHTD

The indirect sulfate emission factor, consisting mainly of ammonium sulfate and ammonium bisulfate is calculated using the following equation:

$$\text{ISULF}_{m,v} = \text{ICNVRT} * \text{SO2}_{m,v} * (3/2) * \text{AMNWGT} \quad (4-88)$$

where:

$\text{ISULF}_{m,v}$  is the indirect sulfate emission factor of a vehicle (grams/mile)

ICNVRT is the fraction of  $\text{SO}_2$  converted to sulfate in the atmosphere (12 percent)

$3/2$  is the weight ratio of  $\text{SO}_2$  to sulfate

AMNWGT is the estimated weight ratio of the combination of ammonium bisulfate and ammonium sulfate in the atmosphere to sulfate (1.6)

#### Total Exhaust Particulate Emission Factors for Gasoline-Fueled Vehicles

The total exhaust particulate emission factors for light-duty gasoline fueled vehicles are calculated by summing lead, direct sulfate, and a carbon emission factor which includes soluble organic material and other remaining carbon. Table 4-5 presents a summary of the carbon emission factors by vehicle model year and type of technology.

Table 4-5. Carbon Emission Factors for Gasoline-Fueled Vehicles (grams/mile)

Vehicle Type/ Model Year	Leaded Fuel	Unleaded/ Catalyst Equipped (No air pump)	Unleaded/ Catalyst Equipped (with air pump)	Unleaded/ Non- catalyst equipped
Light-Duty Gasoline Vehicles				
pre-1970	.193	NA	NA	.030
1970-1974	.068	.0060	.0250	.030
1975-1980	.030	.0060	.0250	.030
1981 +	.017	.0043	.0043	.017

Table 4-5. Carbon Emission Factors for Gasoline-Fueled Vehicles (grams/mile)

Vehicle Type/ Model Year	Leaded Fuel	Unleaded/ Catalyst Equipped (No air pump)	Unleaded/ Catalyst Equipped (with air pump)	Unleaded/ Non- catalyst equipped
Light-Duty Gasoline Trucks I				
pre-1970	.193	NA	NA	.030
1970-1974	.068	.0060	.0250	.030
1975-1986	.030	.0060	.0250	.030
1987 +	.017	.0043	.0043	.017
Light-Duty Gasoline Trucks II				
pre-1979	.370	NA	NA	.054
1979-1986	.068	.0060	.0250	.030
1987 +	.030	.0043	.0043	.017
Heavy-Duty Gasoline Vehicles				
pre-1987	.370	.054	.054	.054
1987 +	.163	.054	.054	.054

#### Total Exhaust Particulate Emission Factors for Diesel-Fueled Vehicles

The total exhaust particulate emission factors are for diesel-fueled vehicle categories and model years ( $E_{FDPM_{m,v}}$ ). The emission factors for heavy-duty vehicles are in units of grams/brake-horsepower hour (g/BHP-hr), which are converted to grams/mile by PART5. The conversion factors and emission factors vary by model year. The emission factors for light-duty diesel vehicles are in units of grams/mile. The total exhaust emission factors given in Table 4-6 are based on high-sulfur fuel. The sulfur content in diesel fuel was reduced in 1993 by EPA regulatory requirements. Consequently, when a the specified calendar year is 1993 or later, PART5 will adjust the exhaust emission factors for lower sulfur fuel. Particulate emission factors for diesel-fueled vehicles are not adjusted for speed.

Table 4-6. Exhaust Particulate Emission Factors for Diesel-Fueled Vehicles

Vehicle Type/ Model Year Group	Exhaust Particulate Emission Factor
Light-Duty Diesel Vehicles (grams/mile)	
pre-1981	.700
1981	.259
1982-1984	.256
1985-1986	.255
1987	.134
1988-1990	.132
1991-1993	.131
1994-1995	.128
1996 +	.100
Light-Duty Diesel Trucks (grams/mile)	
pre-1981	.700
1981	.309
1982-1984	.354
1985-1986	.358
1987	.334
1988-1990	.291
1991-1993	.294
1994-1996	.130
1997 +	.109
Class 2B Heavy-Duty Diesel Vehicles (grams/brake horsepower-hour)	
pre-1988	.5156
1988-1990	.5140
1991-1993	.2873
1994 +	.1011
Light Heavy-Duty Diesel Vehicles (grams/brake horsepower-hour)	

Table 4-6. Exhaust Particulate Emission Factors for Diesel-Fueled Vehicles

Vehicle Type/ Model Year Group	Exhaust Particulate Emission Factor
pre-1988	.5156
1988-1990	.5140
1991-1993	.2873
1994 +	.1011
Medium Heavy-Duty Diesel Vehicles (grams/brake horsepower-hour)	
pre-1987	.6946
1988-1990	.4790
1991-1993	.2747
1994 +	.0948
Heavy Heavy-Duty Diesel Vehicles (grams/brake horsepower-hour)	
pre-1987	.6444
1988-1990	.4360
1991-1993	.2709
1994 +	.0836
Buses (grams/brake horsepower-hour)	
pre-1987	.6931
1988-1990	.4790
1991	.2772
1992 without traps	.1716
1992 with traps	.0257
1993 without traps	.1457
1998 with traps	.0240
1994 +	.0591

Soluble Organic Fraction and Remaining Carbon Portion Emission Factors for Diesel-Fueled Vehicles



The PART5 model calculates the Soluble Organic Fraction (SOF) emission factor as a fraction of the remaining mass, using the following equation:

$$\text{SOF}_{m,v} = [\text{EF}_{m,v} - \text{DSULF}_{m,v}] * (\text{fraction}_{\text{SOF},v}) \quad (4-89)$$

The Remaining Carbon Portion (RCP) is defined the remainder (everything else):

$$\text{RCP}_{m,v} = \text{EF}_{m,v} - \text{DSULF}_{m,v} - \text{SOF}_{m,v} \quad (4-90)$$

where:

- m is the model year of a selected vehicle
- v is the class of a selected vehicle
- $\text{SOF}_{m,v}$  is the Soluble Organic Fraction of the exhaust particulate emission factor (grams/mile)
- $\text{RCP}_{m,v}$  is the remaining carbon portion (elemental carbon) of the exhaust particulate emission factor (grams/mile)
- $\text{EF}_{m,v}$  is  $\text{EFDPM}_{m,v} * \text{CF}_{m,v}$ , the exhaust particulate emission factor for a vehicle (grams/mile)
- $\text{EFDPM}_{m,v}$  is the exhaust particulate emission factor for a vehicle (grams/Brake Horsepower-hour)
- $\text{CF}_{m,v}$  is the conversion factor from grams/Brake Horsepower-hour to grams/mile (Brake Horsepower-hour/mile)
- $\text{fraction}_{\text{SOF},v}$  is the fraction of the non-sulfate portion (ie. the carbon portion) of the diesel exhaust particulate emission factor which is organic carbon for a vehicle (Brake Horsepower-hours/mile)

The Soluble Organic Fractions ( $\text{fraction}_{\text{SOF},v}$ ) for different vehicle classes are as follows (U.S. EPA, 1990):

- 0.18 for LDDVs (Light-Duty Diesel Vehicles)
- 0.50 for LDDT1s (Class 1 Light-Duty Diesel Trucks)
- 0.48 for LDDT2s (Class 2 Light-Duty Diesel Trucks)
- 0.51 for LHDDVs (Light Heavy-Duty Diesel Vehicles) and 2BHDDVs (Class 2B Heavy-Duty Diesel Vehicles)
- 0.44 for MHDDVs (Medium Heavy-Duty Diesel Vehicles) and BUSES
- 0.24 for HHDDVs (Heavy Heavy-Duty Diesel Vehicles)

#### Idle Emission Factors for Heavy Diesel-Fueled Vehicles

Idle emission factor data in grams/hour were collected from manufacturers for heavy-duty diesel vehicle classes only. Consequently, the idle emission factors are not included into the “all vehicles” emission category. The vehicle class emission factors are calculated by averaging together model-year-specific emission data, where the model-year-specific emission data are weighted by the estimated travel fraction of that model year within the vehicle class.

The idle emission factors are model-year-specific but the model year emission rates do not vary by vehicle class. Consequently, the same model year emission factors are used for all the heavy-duty diesel classes, and the differences between idle emission factors between classes reflects only the differing travel fractions between model years for a class. As a result, the emission factors reported for the smaller of the heavy-duty vehicle classes, such as 2BHDDV and LHDDV, may be over estimated. The base idle emission factors in PART5 for all heavy-duty diesel vehicles are as follows:

- 5.370 grams/hour for models prior to 1988
- 3.174 grams/hour for model years 1988-1990
- 1.860 grams/hour for model years 1991-1993
- 1.004 grams/hour for model year 1994 +

#### Re-entrained Dust from Unpaved Roads

Re-entrained road dust emission factors for  $PM_{10}$  (particulate matter less than 10 micrometers in size) in PART5 are estimated using an equation (4-91) based on ambient measurements. Because these measurements include particulate matter from brake wear, tailpipe exhaust, tire wear, and ambient background particulate matter concentrations, these factors must be subtracted from the unpaved road particulate emission factors before the latter factors can be applied. It is necessary to obtain a data base of unpaved and paved road types by county for regional modeling purposes. The MEPPS contains procedures and estimates for 1995 developed for EPA by calculating re-entrained emissions by the month at the state road-type level for the average vehicle fleet, and then allocated to the county road type by population for unpaved roads and by total VMT for paved roads. These procedures should be consulted for more details, such as the means of estimating unpaved and paved VMT data. The equation used to calculate  $PM_{10}$  from unpaved roads is as follows:

$$UNPVD = PSDUNP * 5.9 * (UNSILT/12.0) * (SPD/30.0) * (WEIGHT/3.0)^{0.7} * (VWHEEL/4.0)^{0.5} * (365-IPDAYS)/365 * 453.592 \quad (4-91)$$

where:

- UNPVD is the fleet average unpaved road dust emission factor (grams/mile)
- PSDUNP is the fraction of particles less than or equal to the particle size cutoff (the cutoff is 10 micrometers in MEPPS)
- UNSILT is the percent silt content of the surface material (user input)
- SPD is the average vehicle speed in miles/hour (user input)
- WEIGHT is the fleet average vehicle weight (user input in pounds)
- VWHEEL is the fleet average number of wheels (user input, default is 4)
- IPDAYS is the average number of precipitation days per year with greater than 0.01 inches of rain (user input - MEPPS contains climatological default data for 1995)
- 453.592 is the number of grams in a pound

Emission factors for brake and tire wear (in addition to exhaust emissions) must be calculated so that they may be subtracted from the unpaved road emission factors. The brake wear emission factor is assumed to be the same for all vehicle classes. It is set equal to:

$$\text{BRAKE} = 0.0128 * \text{PSBRK} \quad (4-92)$$

where: PSBRK is the fraction of particles less than or equal to the particle size cutoff. The emission factor 0.0128 grams/mile is taken from U.S. EPA, 1985c.

The tire wear emission factor is calculated using the following equation:

$$\text{EFTIRE}_v = 0.002 * \text{PSTIRE} * \text{IVEHWL}_v \quad (4-93)$$

where: v is a selected vehicle class  
 EFTIRE<sub>v</sub> is the tire wear emission factor  
 0.002 is the emission rate of airborne particulate matter from tire wear for light-duty vehicles (U.S. EPA, 1985)  
 PSTIRE is the fraction of particles less than or equal to the particle size cutoff  
 IVEHWL<sub>v</sub> is the average number of wheels on a vehicle of a given class, where  
 LDGV=4, LDGT1,2=4, HDGV=6, MC=2, LDDV=4, LDDT=4, 2BHDDV=4,  
 LHDDV=6, MHDDV=6, HHDDV=18, BUSES=4

#### Re-entrained Dust from Paved Roads

The PM<sub>10</sub> emission factor for paved roads is estimated similarly to that for unpaved roads. The VMT data for paved roads may be developed following the procedures described in U. S. EPA, 1998. The equation used to estimate paved road re-entrained dust emission factors again is based on ambient measurements, and tailpipe, brake wear, and tire wear emission factors must be subtracted prior to use of the paved road dust emission factor. The paved road emission factors are calculated by:

$$\text{PAVED} = \text{PSDPVD} * (\text{PVSILT}/2.0)^{0.65} * (\text{WEIGHT}/3.0)^{1.5} \quad (4-94)$$

where: PAVED is the fleet average paved road dust emission factor (grams/mile)  
 PSDPVD is the base emission factor for the particle size cutoff (10 micrometers in MEPPS)  
 PVSILT is the road surface silt loading (grams/square meter) (user input)  
 WEIGHT is the fleet average vehicle weight (input by the user in pounds)

#### Application in MEPPS

The PART5 model is a companion of Mobile5a in MEPPS. When running MEPPS interactively through the Tools Manager, the user is prompted to specify input data and options under

EMPRO, Mobile Source Model. Standard lookup data files can be found in the Models-3 directory structure at /home/models3/datasets/nostudies/part5/. Default/example input data sets are included for the 1995 calendar year. When a study is created, the study input data are located at \$EMS\_HOME/project/\$EMS\_PROJECT/raw\_data/\$EMS\_DOMAIN/common/.

If the user is processing mobile emission data using the Study Planner, it is necessary to ensure that the appropriate PART5 input data sets are in place first. This may be accomplished when using MEPPS interactively to establish MEPPS directory structure prior to running through Study Planner. If the data are in place, Study Planner will automatically process them.

When processing mobile particulate emission data, the input and output data of PART5 are assigned to and summed within each grid cell in the same fashion given in detail under the *Gridding VMT* discussion of the implementation of the Mobile 5a model (above).

#### 4.2.5 Chemical Speciation of Emission Data

Chemical transport models, such as CMAQ, require that emission data be provided for either individual species or specific species groups or “lumped” species. This is necessary so that the atmospheric chemistry of pollutants may be more accurately modeled. However, an initial processing step is required because emission data are often reported for pollutants that are aggregates of many species, such as VOC. These aggregate pollutants must be split into their component species, or “speciated”.

The speciation takes two forms, discrete and lumped-model.

In discrete speciation, a pollutant is split into the individual components which comprise the pollutant. For the organic pollutant TOG (total organic gas), the individual components which comprise the pollutant are dependent on a variety of factors including the process, fuel type, and device from which the emissions occurred. For example, TOG from the exhaust of automobile may contain approximately fifty discrete organic compounds (benzene, methane, toluene, hexane, etc.), while TOG from degreasers may contain approximately seventy discrete organic compounds. NO<sub>x</sub> (nitrogen oxides), which is related to combustion processes, is speciated (discrete) into NO and NO<sub>2</sub> (and sometimes HONO).

The discrete components in an emission stream are determined by a number of methods including source testing, surrogate application, and engineering knowledge of the process. Many sources have been inventoried and a compendium of species profiles has been assembled by the US EPA in the *Air Emissions Species Manual* (US EPA, 1988). The *Air Emissions Species Manual* contains a list of TOG and particulate matter (PM) species profiles to which a substantial number of emission sources have been assigned. A compendium of species profiles currently available is compiled in the US EPA *Speciate* database. The database is available on the *Air Chief* CD ROM, which is updated annually (US EPA, 1997). Each of the species profiles identifies the mass percent of the discrete compounds that comprise TOG and PM. Note that NO<sub>x</sub>, SO<sub>x</sub> (sulfur oxides), and CO (carbon monoxide) do not have source-specific speciation

profiles. For all sources,  $\text{NO}_x$  is discretely speciated into NO and  $\text{NO}_2$  (and sometimes HONO), and CO is treated explicitly. The speciation processor currently assumes that  $\text{NO}_x$  is speciated to 95 percent NO and 5 percent  $\text{NO}_2$ , based on average observed values.

The MEPPS EMPRO speciation processor provides chemical speciation of hydrocarbons, oxides of nitrogen, and sulfur oxides. For example, aggregations of hydrocarbon species such as TOG are disaggregated to their component individual chemical species. The processor speciates the spatially and temporally allocated emission estimates that are prepared by the emission estimation processors and models (e.g., point source processor, mobile emission model). The speciation is accomplished using look-up tables of profiles containing source-category specific and specie-specific chemical split factors (percent of mass of source emissions attributable to each specie for a given source category). The general components of emission speciation processing are illustrated in Figure 4-6.

It is computationally prohibitive to model the chemistry of all discrete VOC compounds in the emissions stream in photochemical grid models. Therefore, individual organic species comprising Total Organic Gas are assigned to one or more model species (groups of species) according to the chemical mechanism that is being used. Thus, instead of modeling with a larger number of discrete compounds, the discrete compounds are lumped into a much smaller number of mechanism species. The rules for assigning the discrete compounds to the mechanism species are mechanism dependent and typically involve lumping in one of two ways: 1) lumping compounds with similar reactivity characteristics into a single mechanism species (the lumped molecule approach) or 2) assigning molecular fragments of an individual compound to one or more mechanism species on the basis of molecular structure (lumped structure approach). In Models-3, the lumping of discrete compounds to form mechanism species is carried out using tables of split factors that assign the discrete compounds to mechanism species. Currently, two mechanisms, the Regional Acid Deposition Model 2.0 (RADM2) and Carbon Bond 4 (CB-4) are available in Models-3. The user may also define lumping procedures for an alternative mechanism if the assignment methods for that mechanism are known, or the user may create a modified version of the lumping procedure for one of the two mechanisms in Models-3.

In the CB-4 mechanism, discrete compounds are assigned to mechanism species on the basis of the compound's carbon bond structure (Gery et al., 1989). For instance, single carbon-carbon hydrocarbon bonds are assigned to a paraffin group (PAR), and carbon-carbon double bonds are assigned to an olefinic group (OLE). Thus, an individual discrete VOC could be dis-aggregated into more than one mechanism species depending on its structure. Descriptions of the CB-4 mechanism species are given in Table 4-8.

The RADM2 mechanism lumps discrete compounds on the basis of their prevalence in the atmosphere, common reactivity, and/or molecular weight (Stockwell et al., 1990). For RADM2, individual VOC compounds are first assigned to one of 32 lumped groups. The 32 lumped groups are then further reduced to 15 groups for increased computational efficiency. The relationship between the 32 and 15 lumped groups is shown in Table 4-9. The EMPRO does not

include chemical or size fractionation of particulate matter, although size fractionation of particulate matter is planned in the future.

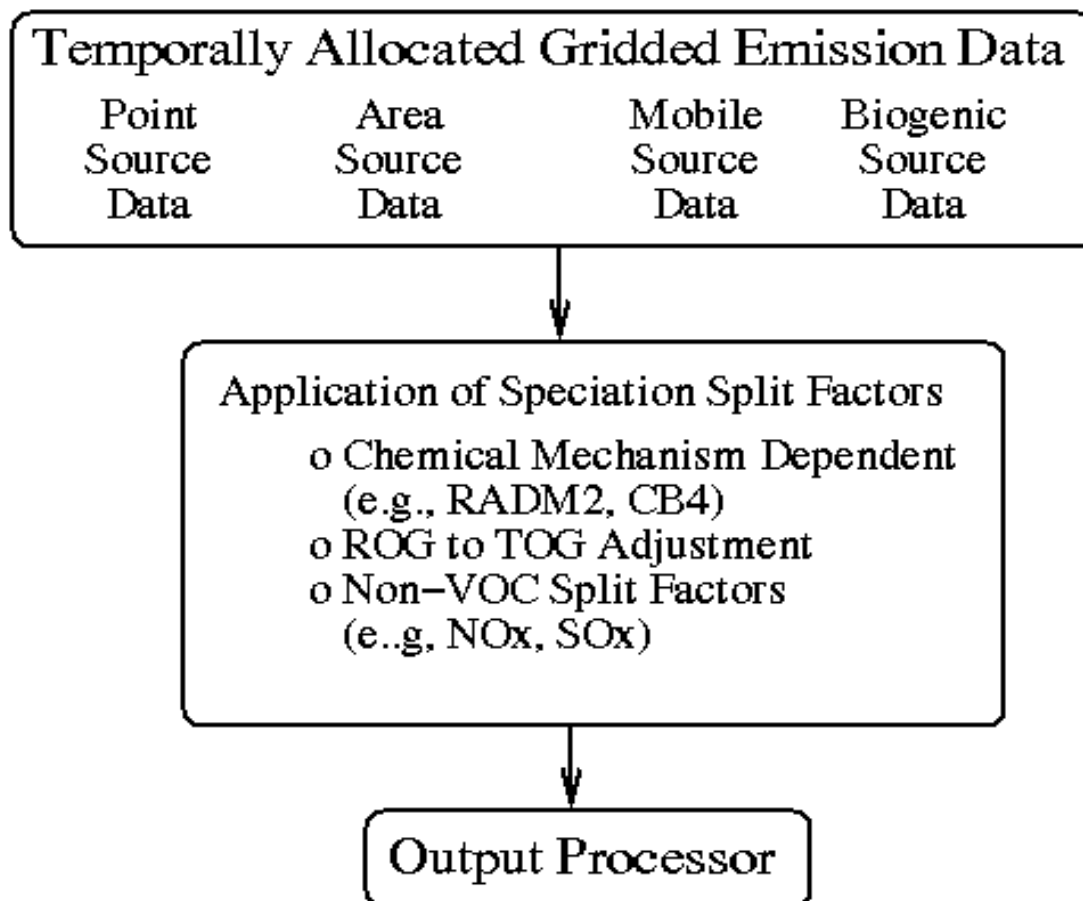


Figure 4-6 General Components of Emission Speciation Processing

Table 4-8. Carbon Bond-4 Lumped Species

CB4 Lumped Species Number	CB4 Lumped Species Code	Lumped Species Description
1	OLE	Olefinic carbon bond (C=C)
2	PAR	Paraffin carbon bond (C-C)
3	TOL	Toluene (C <sub>6</sub> H <sub>5</sub> -CH <sub>3</sub> )
4	XYL	Xylene (C <sub>6</sub> H <sub>4</sub> -(CH <sub>3</sub> ) <sub>2</sub> )
5	FORM	Formaldehyde (CH <sub>2</sub> =O)
6	ALD2	High MW aldehydes (RCHO, R>H)
7	ETH	Ethene (CH <sub>2</sub> =CH <sub>2</sub> )
8	MEOH	Methanol (CH <sub>3</sub> OH)
9	ETOH	Ethanol (C <sub>2</sub> H <sub>5</sub> OH)
10	ISOP	Isoprene
11	NR	Non Reactives as methane
12	NO	Nitric Oxide
13	NO <sub>2</sub>	Nitrogen Dioxide
14	CO	Carbon Monoxide
15	SO <sub>2</sub>	Sulfur Dioxide
16	AERO	Aerosols (PM)

Table 4-9. RADM 2.0 Lumped Species Descriptions

RADM 2.0 32 Lumped Species	RADM 2.0 16 Lumped Species	Allocation Factor (fraction of one)	Reactivity Factor (ratio)	Description of the 32 RADM Lumped Species Before Grouping to 16 Lumped Species
1	CH4	1	1	Methane
2	ETH	1	1	Ethane
3	HC3	1	0.519	Propane
4	HC3	1	0.964	Alkanes (0.25-0.50)
5	HC5	1	0.956	Alkanes (0.50-1.00)
6	HC8	1	0.945	Alkanes (1.00-2.00)
7	HC8	1	1.141	Alkanes (>2.00)
8	HC8	0.91	1.101	Alkane/Aromatic Mix
8	XYL	0.09	1	Alkane/Aromatic Mix
9	OL2	1	1	Ethene
10	OLT	1	1	Propene
11	OLT	1	1	Alkenes (Primary)
12	OLI	1	1	Alkenes (Internal)
13	OLT	0.5	1	Alkenes (Prim/Int Mix)
13	OLI	0.5	1	Alkenes (Prim/Int Mix)
14	TOL	1	0.293	Benzene/Halobenzenes
15	TOL	1	1	Aromatics (<2 react)
16	XYL	1	1	Aromatics (>2 react)
17	CSL	1	1	Phenols and Cresols
18	OLT	0.5	1	Styrenes
18	TOL	0.5	1	Styrenes
19	HCHO	1	1	Formaldehyde
20	ALD	1	1	Higher Aldehydes
21	KET	1	0.253	Acetone
22	KET	1	1	Ketones



Table 4-9. RADM 2.0 Lumped Species Descriptions

RADM 2.0 32 Lumped Species	RADM 2.0 16 Lumped Species	Allocation Factor (fraction of one)	Reactivity Factor (ratio)	Description of the 32 RADM Lumped Species Before Grouping to 16 Lumped Species
23	ORA2	1	1	Organic Acids
24	HC3	1	0.343	Acetylene
25	HC3	1	0.078	Haloalkenes
26	.	1	1	Unreactive
27	HC3	1	0.404	Others (<0.25 react)
28	HC3	1	1.215	Others (0.25-0.5 react)
29	HC5	1	1.075	Others (0.5-1.0 react)
30	HC8	1	1.011	Others (>1.00 react)
31	.	1	1	Unidentified
32	.	1	1	Unassigned

In Models-3, the user initiates speciation by selecting the chemical mechanism to be used for a study in the Study Manager under the Models-3 framework, and within the MEPPS main window under Tools Manager. The procedure is explained in detail in Chapter 6 of *Models-3 Volume 9B: User Manual*. The speciation processor is written primarily in SAS®; however, it includes some FORTRAN programs. ARC/INFO® is not used in the speciation processor.

#### Speciation Processing in MEPPS

In MEPPS, speciated gaseous emissions can be calculated in either of two units – moles/hour or Kg/hour. (Particle emissions are always calculated as Kg/hr.) Emissions in moles are required by the Models-3 CMAQ, but some analyses require that emissions be expressed in mass per unit time. Emissions in mole and mass units are calculated using the following two generic equations:

$$\text{chemest}_{ij} = \sum_p \sum_m \text{hr}_{imp} * 1000 * \text{rogtotog}_{mp} * \text{factor}_{jmp} / \text{divisor}_{jmp} \quad (4-95)$$

where: chemest<sub>ij</sub> is the gridded emissions estimate for hour i and mechanism species j (moles/hour)

$hr_{imp}$  is the gridded hourly emission estimate of pollutant p (NO<sub>x</sub>, SO<sub>x</sub>, CO, PM, NH<sub>3</sub>, or ROG) for hour i and source category m (Kg /hr). The factor of 1000 is used to convert kilograms to grams.

$rogtotog_{mp}$  is a ROG to TOG conversion factor (discussed below)

$factor_{jmp}$  is a mole-based split factor to allocate total emissions of pollutant p from source category m to mechanism species j

$divisor_{jmp}$  is a second conversion factor to allocate total emissions of pollutant p from source category m to mechanism species j

and

$$estKg_{ij} = \sum_p \sum_m hr_{imp} * rogtotog_{mp} * xmass_{jmp} \quad (4-96)$$

where:  $estKg_{ij}$  is the gridded emissions estimate for hour i and mechanism species j (Kg/hour)

$hr_{imp}$  is the gridded hourly emission estimate of pollutant p (NO<sub>x</sub>, SO<sub>x</sub>, CO, PM, NH<sub>3</sub>, or ROG) for hour i and source category m (Kg /hr)

$rogtotog_{mp}$  is a ROG to TOG conversion factor (discussed below)

$xmass_{jmp}$  is a mass-based split factor to allocate total emissions of pollutant p from source category m to mechanism species j

These equations show that emissions for mechanism species are computed by summing the contributions of pollutants from the different source categories that emit that pollutant. As indicated previously, the assignment of a pollutant to a specific mechanism species usually mechanism dependent, although some assignments may be handled the same way in different mechanisms. In Equations 4-95 and 4-96, the terms  $factor_{jmp}$ ,  $divisor_{jmp}$ , and  $xmass_{jmp}$  are mechanism specific apportioning factors that will be defined further below. Note that, in some cases a pollutant will contribute to only one mechanism species, but in other cases a pollutant will contribute to more than one species. For example, emissions of ammonia are always assigned to a model species named NH<sub>3</sub>, but NO<sub>x</sub> is allocated between two mechanism species NO and NO<sub>2</sub>. The details of the allocation procedure for both the RADM2 and CB4 mechanisms will be described further below. First, however, the derivation and use of the  $rogtotog_{mp}$  conversion factor is described.

### ROG-to-TOG Adjustment

The ROG (Reactive organic gas) to TOG conversion portion of the speciation process is selected when the emission inventory is loaded by INPRO (see section 4.2.2). VOC substances deemed non-reactive (e.g., methane and ethane) are often excluded from inventories, and some emission measurement techniques do not capture all discrete compounds in an emission stream (e.g, formaldehyde). The ROG-to-TOG adjustment factor is used to account for those missing components. It is calculated using Equations 4-97 and 4-98:

$$\text{mistog}_m = \sum_k \text{ntsr}_{k,m} \quad (4-97)$$

$$\text{rogtotog}_m = 1.0 / \text{mistog}_m \quad (4-98)$$

where:  $\text{mistog}_i$  is the sum of mass fractions of the discrete VOC compounds deemed non-reactive or not included in an emission inventory for source category  $m$  (grams of missing compound per gram of TOG)  
 $\text{ntsr}_{k,m}$  is the mass fraction of the missing or non-reactive compound  $k$  in the emission stream for source category  $m$   
 $\text{rogtotog}_m$  is the ROG to TOG conversion factor

Note that the  $\text{rogtotog}_{m,p}$  adjustment factor applies only to anthropogenic emissions of VOC, and thus the  $p$  subscript used in Equation 4-95 and 4-96 has been dropped here. In equations 4-95 and 4-96,  $\text{rogtotog}_{m,p}$  is set to 1.0 for all pollutants other than ROG and also set to 1.0 when VOC emissions of biogenic origin are being computed.

#### Carbon Bond 4 (CB4) Speciation Factors

The CB-4 chemical mechanism is widely used in air quality model simulations of ozone concentrations at urban and regional spatial scales. As described in the introductory part of this section, the basis of the CB-4 mechanism is that reactivity of organic compounds in the atmosphere can reasonably be simulated by mechanism species that represent different carbon bond types. A detailed description of the CB-4 mechanism is contained in Section 8.2.1. The focus of the discussion here is on how the CB-4 apportioning factors used in Equations 4-95 and 4-96 are calculated. Since speciation of anthropogenic VOC emissions is done differently than for other pollutants, the discussion is divided into two subsections.

**Anthropogenic VOC speciation.** For the CB4 mechanism, the apportioning factor  $\text{divisor}_{j,\text{imp}}$  in equation 4-95 is set to 1.0 for all anthropogenic VOC emission calculations (i.e., it is essentially not used). The  $\text{factor}_{j,\text{imp}}$  term for anthropogenic VOC is set equal to a split factor term  $s_{j,l}$  that is computed for a specified VOC emission profile  $l$ , which in turn is assigned to a source category  $m$  (i.e., an SCC or ASC). The split factor for each profile and mechanism species is computed as follows:

$$\text{sf}_{j,l} = \sum_k \text{xmf}_{k,l} / \text{mw}_k * \text{xnum}_{j,k} \quad (4-99)$$

where:  $\text{sf}_{j,l}$  is a molar split factor for CB4 species  $j$  and VOC profile  $l$  (moles of CB4 species/gram of TOG)  
 $\text{xmf}_{k,l}$  is a mass fraction of discrete VOC compound  $k$  in VOC profile  $l$  (grams of discrete VOC/grams of TOG)  
 $\text{mw}_k$  is the molecular weight of discrete VOC compound  $k$  (grams of discrete VOC/mole of discrete VOC)

$xnum_{j,k}$  is the moles of discrete VOC compound  $k$  assigned to CB4 species  $j$  (moles of CB4 species/mole of discrete VOC)

In Equation 4-96, the  $xmass_{j,imp}$  term apportions mass emissions to CB4 species for a given pollutant and source category. Analogous to the CB4 molar split factor defined above, the  $xmass_{j,imp}$  term is set equal to a mass split factor that apportions the mass of a discrete VOC compound according to the fraction of carbon atoms that is assigned to a mechanism species:

$$xmass_{j,l} = \sum_k ( xmf_{k,l} * cn_j ) / cn_k \quad (4-100)$$

where:  $xmass_{j,l}$  is the mass split factor for CB4 species  $j$  and VOC profile  $l$  (moles of CB4 species/gram of TOG)  
 $xmf_{k,l}$  is the mass fraction of discrete VOC compound  $k$  in VOC profile  $l$  (grams of discrete VOC/grams of TOG)  
 $cn_j$  is the number of carbon atoms in CB4 species  $j$   
 $cn_k$  is the number of carbon atoms in discrete VOC compound  $k$

Again, one VOC profile is assigned to each source category, and thus split factors are generated for each source category/mechanism species combination.

Other speciation. For pollutants and source categories other than anthropogenic VOC, the terms  $factor_{j,imp}$ ,  $divisor_{j,imp}$ , and  $xmass_{j,imp}$  are simply assigned numeric values that determine the allocation of pollutant emissions. These are summarized in Table 4-10.

For all pollutants (except particles) in Table 4-10, the divisor corresponds to the molecular weight of the pollutant and is used in equation 4-76 to convert mass emissions of the pollutant to moles of pollutant. The two split factors  $factor_{j,imp}$ , and  $xmass_{j,imp}$  are used to apportion the pollutant emissions to the mechanism species. A factor of 1.0 indicates a 1:1 correspondence. Factors different from one indicate a disaggregation or lumping of pollutant emissions into individual species.

CO and NH<sub>3</sub> are treated explicitly in many air quality models, and therefore emissions of these compounds are not split into other components. Similarly, particle emissions are treated explicitly so no lumping or dis-aggregation is necessary for them either.

When SO<sub>x</sub> emissions are speciated, 97% of the SO<sub>x</sub> mass is treated as SO<sub>2</sub>. The remaining 3% of the SO<sub>x</sub> mass corresponds to SO<sub>4</sub> (or SULF), but is dropped from further consideration. SO<sub>2</sub> and SO<sub>4</sub> emissions are treated as explicit species.

Table 4-10. CB4 Split Factors for Pollutants Other Than Anthropogenic VOC

Source Category	Pollutant	CB4 Species	factor <sub>jmp</sub>	divisor <sub>jmp</sub>	xmass <sub>jmp</sub>
All	CO	CO	1.0	28.0	1.0
All	NH3	NH3	1.0	17.0	1.0
All	AERO	AERO	1.0	1.0	1.0
All	PM10	PM10	1.0	1.0	1.0
All	PM2_5	PM2_5	1.0	1.0	1.0
All except BIO	NOX	NO	0.62	30.0	0.62
All except BIO	NOX	NO2	0.05	46.0	0.05
All	SO2	SO2	1.0	64.0	1.0
All	SOX	SO2	0.97	64.0	0.97
All	SO4	SULF	1.0	96.0	1.0
BIO	NO	NO	1.0	30.0	1.0
BIO	Isoprene	ISOP	1.0	68.12	1.0
BIO	OVOC	NR	0.5	148.0	0.05
BIO	OVOC	OLE	0.5	148.0	0.10
BIO	OVOC	PAR	8.0	148.0	0.85
BIO	TERP	ALD2	1.5	136.23	0.3
BIO	TERP	OLE	0.5	136.23	0.1
BIO	TERP	PAR	6.0	136.23	0.6
BIO	TERP	TERPB	1.0	136.23	1.0

In MEPPS, it is assumed that NO<sub>x</sub> is composed of 95% NO and 5% NO<sub>2</sub> (by mass). However, actual NO<sub>x</sub> composition can vary from 89%/11% to 95%/5%. In a few cases, a small percentage (<2%) of NO<sub>x</sub> emissions is assumed to be nitrous acid (HONO). Since NO<sub>x</sub> emissions are typically reported as NO<sub>2</sub> mass, it is necessary to normalize the NO<sub>x</sub> emissions by the molecular weight of NO<sub>2</sub>. Hence, the molar split factors (factor<sub>jmp</sub>) for NO and NO<sub>2</sub> are calculated as follows:

$$sf_{NO} = xmf_{NO} * mw_{NO} / mw_{NO2} \quad (4-101)$$

$$sf_{NO_2} = xmf_{NO_2} * mw_{NO_2} / mw_{NO_2} \quad (4-102)$$

With a NO<sub>x</sub> composition of 95% NO (as NO<sub>2</sub>) and 5% NO<sub>2</sub> by mass, the split factors for NO and NO<sub>2</sub> become 0.62 and 0.05, respectively. The mass split factors are calculated in the same manner, and thus have the same values as for the molar split factors.

The speciation of biogenic emissions in CB4 is the same as used in the Regional Oxidant Model (EPA, 1989). Isoprene is treated as an explicit species and terpene emissions are speciated into 1.0 mole of OLE, 6.0 moles of PAR, and 3.0 moles of ALD2. Terpenes are also assigned to the model species TERPB for special processing in the aerosol module of the CMAQ. The apparent double counting of terpene emissions is accounted for in the CMAQ processing however. Finally, the category OVOC (other VOCs from biogenic sources) is apportioned to 1.0 mole of OLE, 8.5 moles of PAR, and 0.5 mole of NR. Here it assumed that number of carbon atoms in a OVOC molecule is 10.

### RADM2 Speciation Factors

The RADM2 chemical mechanism was developed for and has been used principally in regional air quality simulations of sulfur dioxide (SO<sub>2</sub>) and oxides of nitrogen for acid rain assessment (Walters and Saegar, 1990). A detailed description of the RADM2 mechanism is given in section 8.2.2. The speciation procedure used for RADM2 is fully described in Walters and Saeger (1990), and will only be summarized here. This section focuses on how the RADM2 apportioning factors used in Equations 4-95 and 4-96 are calculated. Again, the discussion is divided into two subsections, one dealing with the speciation of anthropogenic VOC emissions and one with all other speciation.

**Anthropogenic VOC speciation.** The RADM2 mechanism requires that discrete organic VOC compounds be lumped into 15 mechanism species based on common reactivity and reaction products. As with the CB4 mechanism, the apportioning factor divisor<sub>jmp</sub> in Equation 4-95 is set to 1.0 for all anthropogenic VOC emission calculations, and thus is not used. Also as with the CB4 mechanism, The factor<sub>jmp</sub> term for anthropogenic VOC is set equal to a split factor term  $s_{ji}$  that is computed for a specified VOC emission profile  $l$ , which in turn is assigned to a source category  $m$  (i.e., an SCC or ASC). However, the RADM2 split factors are calculated using the following equation:

$$sf_{j,l} = \sum_k xmf_{k,l} * afac_{j,k} * rfac_{j,k} / mw_k \quad (4-103)$$

where:  $sf_{j,l}$  is the molar split factor for RADM2 species  $j$  and VOC profile  $l$  (moles of RADM2 species/gram of TOG)  
 $xmf_{k,l}$  is the mass fraction of discrete VOC compound  $k$  in VOC profile  $l$  (grams of discrete VOC/grams of TOG)

$afac_{j,k}$  is the allocation factor listed in Table 4-6 for RADM2 species  $j$  and discrete VOC compound  $k$

$rfac_{j,k}$  is the reactivity factor listed in Table 4-6 for RADM2 species  $j$  and discrete VOC compound  $k$

$mw_k$  is the molecular weight of discrete VOC compound  $k$  (grams of discrete VOC/mole of discrete VOC)

In the RADM2 speciation process, each discrete VOC compound is assigned to one of the 32 lumped species categories, and that assignment is used to further lumped to one of the 15 species in the condensed group. See Middleton et al. (1990) for information on how the allocation and reactivity factors are derived.

In Equation 4-96, the term  $xmass_{j,imp}$  apportions mass emissions to RADM2 species for a given pollutant and source category. Analogous to the RADM2 molar split factor defined above, the term  $xmass_{j,imp}$  is set equal to a mass split factor that apportions the mass of a discrete VOC compound according to the mass fraction of the discrete VOC compound in the emission stream and the mechanism specific allocation factor:

$$xmass_{j,l} = \sum_k xmf_{k,l} * afac_{k,l} \quad (4-104)$$

where:  $xmass_{j,l}$  is the mass split factor for RADM2 species  $j$  and VOC profile  $l$  (moles of CB4 species/gram of TOG)  
 $xmf_{k,l}$  is the mass fraction of discrete VOC compound  $k$  in VOC profile  $l$  (grams of discrete VOC/grams of TOG)  
 $afac_{j,k}$  is the allocation factor listed in Table 4-6 for RADM2 species  $j$  and discrete VOC compound  $k$

Other speciation. For pollutants and source categories other than anthropogenic VOC, the terms  $factor_{j,imp}$ ,  $divisor_{j,imp}$ , and  $xmass_{j,imp}$  are simply assigned numeric variables that control the allocation of emissions, similar to what is done for the CB4 mechanism. The factors for RADM2 are summarized in Table 4-11.

Except for the biogenic categories, the contents of Table 4-11 are identical to those in Table 4-10 for the CB4 mechanism. Thus, the reader is referred to the corresponding CB4 section for information on those source category/pollutant combinations. The biogenic portions of the two tables are similar in that isoprene is treated as an explicit species in RADM2, and terpenes and other VOCs (OVOC) of biogenic origin are apportioned to mechanism species. In RADM2, terpenes are apportioned entirely to OLI (Middleton et al., 1990). As with the CB4 mechanism, terpenes are also assigned to the model species TERPB for special processing in the aerosol module of the CMAQ, but the apparent double counting of terpene emissions is accounted for in the CMAQ processing however. Finally, the assignment of other VOC species to RADM2

species is carried out in a manner analogous to that for CB4: 85% is assumed to correspond to slow reacting alkanes, 15% to fast reacting olefins, and 5% is assumed to be non-reactive. Thus, in RADM2 85% of the OVOC mass is assigned to the category containing the slowest reacting alkanes (category 27 in Table 4-6). The split factor is obtained by multiplying the mass fraction (.85) by the reactivity factor (0.404) to give a molar split factor of 0.343. The 10% of the mass of OVOC assumed to be reactive olefins is assigned to the OLI category. Both the mass and molar split factors for this compound are simply 0.1.

Table 4-11. RADM2 Split Factors for Pollutants Other Than Anthropogenic VOC

Source Category	Pollutant	CB4 Species	factor <sub>jmp</sub> *	divisor <sub>jmp</sub> *	xmass <sub>jmp</sub>
All	CO	CO	1.0	28.0	1.0
All	NH3	NH3	1.0	17.0	1.0
All	AERO	AERO	1.0	1.0	1.0
All	PM10	PM10	1.0	1.0	1.0
All	PM2_5	PM2_5	1.0	1.0	1.0
All except BIO	NOX	NO	0.62	30.0	0.62
All except BIO	NOX	NO2	0.05	46.0	0.05
All	SO2	SO2	1.0	64.0	1.0
All	SOX	SO2	0.97	64.0	0.97
All	SO4	SULF	1.0	96.0	1.0
BIO	NO	NO	1.0	30.0	1.0
BIO	Isoprene	ISO	1.0	68.12	1.0
BIO	OVOC	HC3	0.343	148.0	0.85
BIO	OVOC	OLI	0.1	148.0	0.1
BIO	TERP	OLI	1.0	136.23	1.0
BIO	TERP	TERPB	1.0	136.23	1.0

#### 4.2.6 Output Processor (OUTPRO)

The results of MEPPS processing must be in a form that is useful to the Models-3 framework and readily evaluated for the substantive content and quality of the data. The OUTPRO processes spatially and temporally allocated, speciated emission data files to prepare them for use by the Models-3 framework and its components, including CMAQ. In addition, OUTPRO prepares many standard and user-defined emission summary reports. The processing includes the following items:



- Merging of temporally allocated point, area, biogenic, and mobile source emission data files.
- Merging of speciated point, area, biogenic, and mobile source emission data files .
- Merging of point, area, biogenic, and mobile source files into a consolidated two-dimensional emission file. Merging is optional; and data type files may be maintained and output separately.
- Preparation of three-dimensional point source emission files for use by the plume rise and Plume-in-Grid models available in CMAQ. The user may define groups of similar stacks by specifying percentage tolerance differences in different physical stack properties. In addition, the user may categorize minor, major, and major elevated point source emission (MEPSE) stacks by their emission rates and/or stack properties . The classification criteria are not pre-specified, but are set by the user. Specifically, any combination of emissions of specified pollutants in tons/day and/or physical stack parameters including height, diameter, flow rate, or exhaust velocity may be used to define a major or MEPSE point source. Generally, MEPSE stacks are the largest of point sources, such as electric utility stacks. Major point sources are usually somewhat smaller, but significant point sources. Source-specific information is necessary to classify MEPSE or major point sources. Smaller sources not classified as MEPSE or major point sources or without source-specific information are referred to as minor point sources, and are usually included with the surface area sources by OUTPRO, unless specified otherwise by the user.
- Conversion of output file format to NetCDF I/O API format. This allows other components of the Models-3 framework, including the CMAQ and visualization tools, to use the emission files. The CMAQ accepts the emission files and processes them for input to CMAQ using the Emission Chemical Input Processor (ECIP). The ECIP is described in Section 7.
- Preparation of summary reports of the processed emission files, including summaries by primary emission type (point, area, biogenic, mobile), by geographic area (grid area, grid cell, state, county, etc.), by source category code and groups of codes (tiers, or combinations of these items. In addition, the reports rank emission values by amount, type, geographic area, etc.

### **4.3 Models-3 Emission Projection Processor (MEPRO)**

It is often necessary to iteratively project emissions and emission control combinations to future years in order to model future year ambient pollutant concentrations relative to regulatory standards. Consequently the Models-3 system includes a projection and control system, the Models-3 Emission Projection (MEPRO) processor to perform the necessary work. The MEPRO was developed from the Multiple Projection System (MPS). The MPS was originally designed as a stand-alone software tool to assist the EPA in projecting and tracking the "reasonable further progress" of regulatory emission reduction programs for criteria pollutants (Monroe et al., 1994). It may be invoked from Strategy Manager from the Models-3 framework or run separately. Because MPS was designed as a PC application using the Superbase<sup>®</sup> programming language, MEPRO must be run under an emulator (SoftWindows<sup>®</sup>) if it is used in an UNIX operating system. Currently, MEPRO is more efficiently run on a PC workstation with a Windows NT<sup>®</sup> operating system. Figure 4-7 illustrates the relationship of MEPRO with the rest of MEPPS.

Using MEPRO, the user may edit regulatory control factors, control efficiency, rule penetration, rule effectiveness, as well as "across-the-board" emission adjustments and source category code-specific emission projections. Projected emission inventory data, and/or inventory data with revised emission controls and efficiencies are passed to EMPRO (in the `/raw_data/$EMS_DOMAIN/common/` directory) for processing to the NetCDF I/O API format required for air quality modeling by CMAQ. Mobile source emissions are not projected in MEPRO. Instead, VMT is projected, and the projected mobile sources emissions are computed in the mobile source model of EMPRO.

The MEPRO will project emissions of NO<sub>x</sub>, VOC, and CO for each year from 1991 through 2010, using the 1990 EPA inventory for the base year. The capability to project SO<sub>2</sub> and PM emission data may be provided in the future. Projections are by source category code of emissions for any area in the United States. The base year and the annual projection factors will be updated as new data become available. The annual growth factors for VOC, NO<sub>x</sub>, and CO are taken from look-up tables containing economic growth factors by county for the United States. The growth factors are based on economic forecasts applied to specific source category codes by the Economic Growth Analysis System (EGAS) (US EPA, 1995a).

The EGAS system is a PC-based tool which uses a hierarchical three-tiered approach to generate growth factors. Tier 1 is the National Economic Tier. It includes an economic model by Regional Economic Models, Inc (REMI) (Treyz et al., 1994) which is primarily based on the Bureau of Labor Statistics (BLS) American Workforce 1992-2005 projections. After 2005, the BLS moderate growth labor force participation rates and the Census Bureau's middle population projections for the United States are used to forecast the labor force. The second tier is the Regional Economic Tier, the results of which are overlain on the Tier 1 results. The Regional Economic Tier contains separate economic models developed by REMI for each non-attainment area and attainment area of each state. The largest area addressed by one model is a state. The third tier is the Growth Factor Tier, which contains commercial, residential, industrial, and electric utility models, and a VMT growth module. The commercial, residential, and industrial energy models were developed by the Argonne National Laboratory and were used in the

National Acid Precipitation Assessment Program (Boyd et al., 1990). Electrical Utilities projection was accomplished using the Neural Network Electric Utility Model (EUMOD). The default economic projection tables from EGAS are based on U.S. Bureau of Labor Statistics forecasts. Projection factor tables based on forecasts by the Wharton School of Economics are provided as an option.

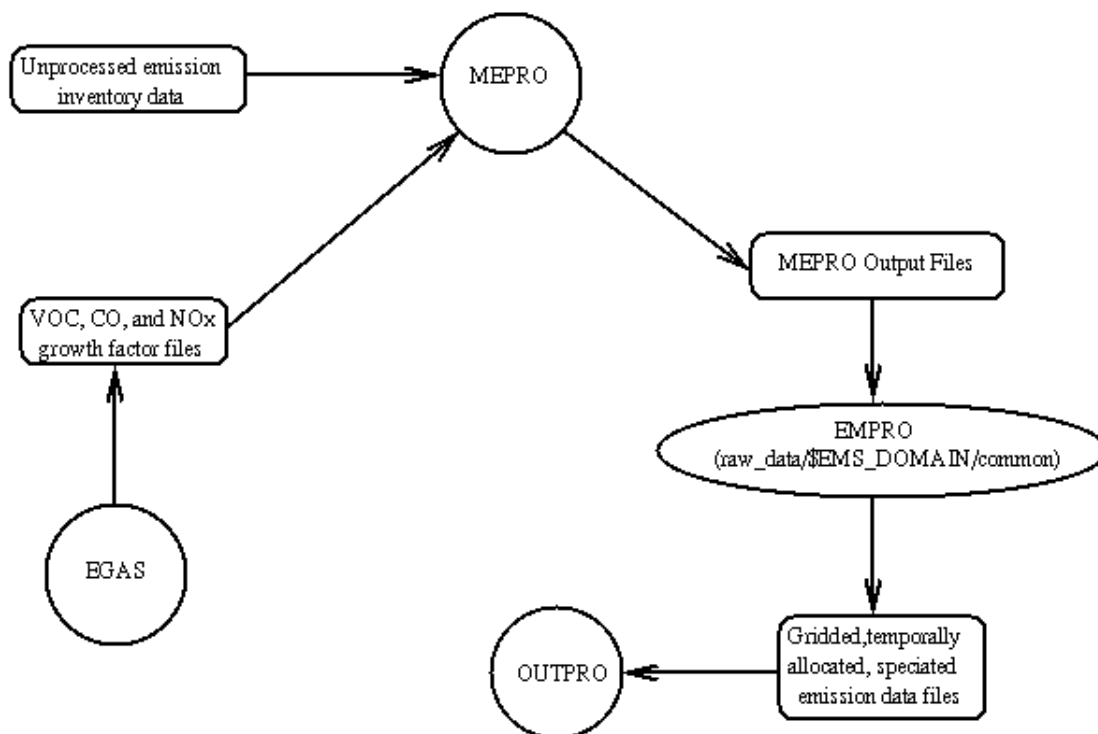


Figure 4-7 MEPRO Relationship to Other MEPPS Components

The method of applying regulatory and growth projection factors to point and area source emission data to obtain future year daily controlled emission data is summarized by Equation 4-105. Because MEPRO projects only the VMT data for mobile source emissions, the projection method is slightly different (Equation 4-106). The projected VMT data are passed to the EMPRO mobile-source emission model to be converted into projection mobile source emission data.

$$\text{PCONE} = \text{DCONE} * \text{PGF} * (1 + \text{AF}/100) * [1 - (\text{PCE} * \text{PRE} * \text{PRP})] / [1 - (\text{CE} * \text{RE} * \text{RP})] \quad (4-105)$$

where: PCONE is the point or area source future-year daily controlled emissions  
DCONE is the base year daily-controlled emissions

PGF is the projected year growth factor (percent)  
 AF is the projected year emission adjustment factor (percent)  
 PCE is the projected year control efficiency  
 PRE is the projected year rule effectiveness  
 PRP is the projected year rule penetration  
 CE is the (adjusted) base year control efficiency  
 RE is the (adjusted) base year rule effectiveness  
 RP is the (adjusted) base year rule penetration

For mobile source data:

$$FPE = BVMT * EF * PGF * (1 + AF/100) \quad (4-106)$$

where: FPE is the future projected emissions (on-road mobile)  
 BVMT is the base VMT by vehicle class by facility class by year  
 EF is the emission factor  
 PGF is the projected year growth factor  
 AF is the projected year emission adjustment factor

Additional details for EGAS and MPS are given the references cited above.

## 4.4 Emission Processing Interface

An accurate characterization of the spatial and temporal variability of emissions at the surface and aloft is vital for realistic air quality grid modeling. The MEPPS creates separate emission files for surface area and elevated point sources for a particular domain and time period to be modeled. Consequently, an interface processor program was needed to efficiently consolidate these various emissions types into a single, hourly gridded data file for use in grid model simulations.

### 4.4.1 Overview of Key Features of ECIP

The Emission-Chemistry Interface Processor (ECIP) serves as the key link between the MEPPS system and the CMAQ Chemistry Transport Model (CCTM). The primary function of ECIP is to generate an hourly 3-dimensional (3-D) emission data file for the CCTM from the individual emission file types produced by the MEPPS.

The schematic diagram in Figure 4-8 shows the principal input files used to drive ECIP. The notable elevated point sources were likely separated into major and MEPSE (Major Elevated Point Source Emissions) source groups, based on a user-specified emission rate criterion during MEPPS processing. The MEPSE group contains the largest point source emissions and is intended to be specially simulated by the CCTM Plume-in-Grid (PING) treatment. However, the PING treatment is an optional capability of the CCTM and when it is not exercised, the MEPSE emission file must be processed by ECIP for the modeling scenario so that the significant

emissions from these point sources are included in the 3-D emission data file with the other major point source emissions. Thus, this capability to include or omit the MEPSE emissions in ECIP allows for CCTM runs to be performed without PING or with the PING treatment, respectively, while not requiring separate runs of the MEPPS emissions system. A companion stack parameter file for each point source emission file is needed by ECIP for plume rise calculations. In addition, meteorological data files generated by MCIP are also required to run ECIP in order to simulate point source plume processes. The ECIP 3-D emission file displayed in Figure 4.6 contains the surface area anthropogenic and biogenic emissions, and the elevated emissions from major point sources and the MEPSEs, if appropriate. The 3-D emissions output file from ECIP is ready for direct input into the CCTM.

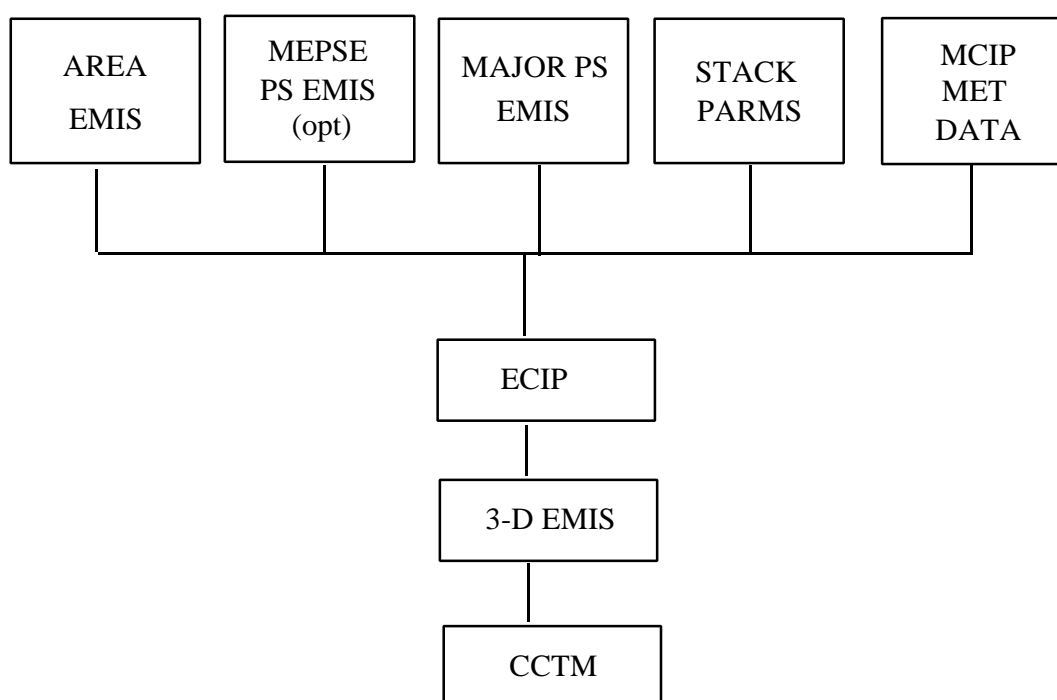


Figure 4-8 Schematic Flow Diagram of the Input Files and 3-D Emission Data File for CCTM generated by ECIP

A specific set of tasks is performed by ECIP for preparation of the 3-D emission file. The 2-D gridded area emissions are incorporated into the first model layer since they represent near-surface releases. In contrast, each elevated point source plume must be subjected to plume rise and initial vertical spread processes prior to the allocation of the plume emissions into the proper grid cells aloft. Another capability of ECIP can be applied in case the CCTM domain is smaller than the emission domain. ECIP can perform "spatial windowing" of the emissions needed for a particular CCTM domain from a larger MEPPS emissions domain.

The methods used in ECIP to treat the processes impacting point source plumes are described in subsequent sections. While these approaches employ existing scientific techniques, it is recognized that other formulations exist. However, the modular design of the Models-3 coding structure allows for the implementation and application of alternative algorithms to treat a particular process.

#### 4.4.2 Plume Rise of Point Source Emissions

The rise of a buoyant plume above stack height is strongly dependent upon the initial stack parameters and atmospheric vertical structure at the time of release. A realistic determination of the height of final plume rise is important to incorporating the plume emissions into the proper vertical layer(s) of the model. The initial buoyancy flux ( $F_b$ ), which is a key parameter in plume rise formulas, is given by

$$F_b = \frac{g(T_s - T_a)(V_s d^2)}{4T_s} \quad (4-107)$$

where  $T_s$  and  $T_a$  are the stack exit temperature and ambient temperature at stack top, respectively. Other notable stack parameters in Equation 4-107 include the plume exit velocity ( $V_s$ ) and stack diameter ( $d$ ), while  $g$  is gravity. Clearly, the magnitude of  $F_b$  is greatly influenced by these stack exit parameters. For buoyant plumes, which exist for the vast majority of point sources,  $F_b$  is greater than zero since  $T_s > T_a$ . However, if  $T_s < T_a$ , then  $F_b$  is set to zero.

The vertical profile of wind and temperature also greatly impact plume rise. In particular, advances in the accuracy of plume rise estimates have resulted from taking into consideration the vertical variations in the thermal stability and wind structure which frequently display a strong height dependency in the atmosphere. A key atmospheric stability parameter ( $s$ ) used to distinguish the different stability regimes aloft is defined by

$$s = (g/T_a)(d\theta/dz) \quad (4-108)$$

where  $d\theta/dz$  is the vertical potential temperature gradient. The value of  $s$  is employed as a criterion to apply the appropriate stability-dependent plume rise formula. However, for the initial calculation of plume rise, the convective velocity scale ( $H_*$ ) is used as an indicator variable to identify the particular stability regime and it is defined by

$$H_* = \frac{g}{T_s} \overline{wT} \quad (4-109)$$

where  $T_s$  is the 1.5m air temperature, and  $wT$  is the surface heat flux covariance. Unstable conditions are defined for  $H_* > 0.03H_{*min}$ , while stable conditions exist when  $H_* < -0.03H_{*min}$ . Neutral conditions occur for the range of values between these criteria. The default value of  $H_{*min}$  has been set to  $10^{-4} \text{ m}^2/\text{s}^3$ .

The layer-by-layer approach described by Turner (1985), as originally suggested by Briggs (1975), has been applied in ECIP for the determination of final plume rise ( $\Delta h$ ) based on the stability of each vertical layer. This practical scheme takes advantage of the vertical resolution of the hourly, temperature and wind profiles and other 2-D meteorological parameters provided by the MM5 dynamic mesoscale meteorological model outputs as postprocessed through MCIP. The method, as outlined by Turner (1985), is an iterative approach which computes plume rise through each layer. An initial plume rise calculation is performed using meteorological variables derived at the stack top height with a stability-dependent plume rise formula at this level. Two methods, linear interpolation or a surface similarity scheme by Byun (1990), are available for deriving temperature and wind at stack height from the modeled profile values. For tall stacks, negligible differences were found in the derived values between these methods. If the projected effective plume rise height ( $h_e = h_s + \Delta h$ ) exceeds the top of the layer containing the stack top, the amount of rise is limited to the height of the current layer top. Then residual buoyancy flux ( $F_R$ ) is determined with an inverted form of the plume rise equation just applied. Using  $F_R$ , the procedure is repeated to determine the plume rise using the profile parameters for the next higher layer. This method is applied over successive layers until the buoyancy flux is completely exhausted. The plume rise ceases at the level where  $F_b = 0$ .

A set of analytical plume rise equations presented by Briggs (1984) for different atmospheric stabilities have been utilized in ECIP for all point sources. The various plume rise equations are provided below. The final effective plume centerline height ( $h_e$ ) is found by adding the computed plume rise ( $\Delta h$ ) to  $h_s$ .

#### 4.4.2.1 Plume Rise Treatment for Stable Conditions

For stable atmospheric conditions, plume rise is taken from Briggs (1984) equation for bent-over plumes.

$$\Delta h = 2.6 \left[ \frac{F_b}{u s} \right]^{1/3} \quad (4-110)$$

where  $u$  is the wind speed for the layer. Equation 4-88 is applied when  $H_* < -0.03H_{*min}$  for the initial plume rise computation at the stack, and when  $s > 10^{-5}$  for subsequent layers in the current approach.

#### 4.4.2.2 Plume Rise Treatment for Unstable Conditions

The plume rise formula proposed by Briggs (1984) during unstable conditions is given by

$$\Delta h = 3[F_b/u]^{3/5} H_*^{-2/5} \quad (4-111)$$

However, Briggs (1983) suggested a reasonable approximation for  $H_*$  which permits Equation 4-111 to be applied in the following form.

$$\Delta h = 30 [F_b/u]^{3/5} \quad (4-112)$$

The rationale for the simplification is due to the lack of data for evaluation to justify a more complicated form. Equation 4-112 is applied with  $H_* > 0.03H_{\min}$  for the first plume rise computation at the stack and for higher layers for  $s < 10^{-5}$ .

#### 4.4.2.3 Plume Rise Treatment for Neutral Conditions

The neutral formula developed by Briggs (1984) plume rise equation has been modified into the following expression.

$$\Delta h = 1.2[F_b/(u u_*^2)]^{3/5} [h_s + 1.3F_b/(u u_*^2)]^{2/5} \quad (4-113)$$

where  $u_*$  is the surface friction velocity. Equation 4-113 introduces minor differences from the other form. Equation 4-113 is a more computationally efficient form suggested by Briggs (1983, communication) since his original neutral formula requires iteration to solve. In the plume rise algorithm of ECIP, the neutral plume rise equation is also solved during other stability conditions in the layers aloft. A comparison between the two plume rise estimates is made and the lower value is selected before proceeding.

#### 4.4.2.4 Special Conditions

For the cases when  $F_b = 0$ , plume rise can occur due to momentum provided by the exit velocity of the plume out of the stack. Therefore, a momentum rise formula (Turner, 1985) has also been implemented to consider these situations and is given by

$$\Delta h_m = 3d v_s/u \quad (4-114)$$

If Equation 4-114 is selected, no further plume rise computations are performed.



Another situation occurs when the stack is below the PBL height ( $z_i$ ) under unstable conditions and the condition  $(h_s - z_i) < 200$  m applies. A treatment for limited plume penetration above the PBL is determined when this situation is triggered. This condition most often occurs during the morning period. Since  $z_i$  is generally growing rapidly, this period is generally brief. To consider plume penetration of the overlying stable layer, a practical algorithm employed previously by Byun and Binkowski (1991) has been implemented based on Briggs (1984). If  $h_s$  is less than 200 m below  $z_i$ , then the following equation is solved.

$$z_b = 3.9[F_b/us]^{1/3} \quad (4-115)$$

If  $z_i$  is greater than  $z_b$ , then the plume top height ( $z_t$ ) is set to  $z_i$  and  $h_e$  is defined to be  $2/3z_t$ . However, plume penetration is permitted when  $z_i < z_b$  in Equation 4-115. For this case, the plume top height is defined to be the height of the top of the next higher layer and the effective plume height is again computed as  $2/3h_t$ .

#### 4.4.3 Method for the Treatment of Initial Vertical Plume Spread

Buoyancy-induced turbulence promotes plume expansion during the rise phase. A widely-used method from Briggs (1975) designates the vertical thickness of a plume to be equivalent to the amount of plume rise. With this method, the heights of the top and bottom of the plume are determined by

$$\begin{aligned} h_t &= h_s + 1.5\Delta h \\ h_b &= h_s - 0.5\Delta h \end{aligned} \quad (4-116)$$

where  $h_t$  and  $h_b$  are the heights of the plume top and bottom, respectively. Since the plume thickness is directly related to the amount of plume rise, this approach leads to rather thick plumes during the nocturnal period. Experimental plume dimension data suggest more limited vertical thickness for plumes during the nighttime hours. As an alternative, an empirical form has also been included. It is based on analyses of observed plume dimensions and vertical temperature gradients (Gillani, 1996 communication). He found the best-fit empirical result is given by

$$\sigma_z = A e^{(-BdT/dz)} \quad (4-117)$$

where the standard deviation of plume depth ( $\sigma_z$ ) is a function of the vertical temperature gradient ( $dT/dz$ ) at  $h_e$ . Values for  $A$  and  $B$  are given by 10 and 117, respectively. A minimum value specified for  $\sigma_z$  is 3 m. With this method,  $h_t$  and  $h_b$  are determined to be  $\pm 2.15\sigma_z$  above

and below  $h_s$ , respectively. This approach provides for smaller plume thicknesses during the nocturnal period.

#### 4.4.4 Vertical Allocation of Plume Emissions

Rather than dumping the entire emissions of a plume into a single layer, an approach has been developed to allow for the allocation of plume emissions into multiple layers since a plume can often span more than one layer. This situation occurs often as more vertical layers are used in the model since model layers are thinner.

Once  $h_t$  and  $h_b$  have been computed for each plume, these values, along with the heights of the model layer interfaces ( $z_z$ ) are employed to determine the fractional amount of plume overlap across each layer. The method uses the fractional amount of the plume depth residing within a layer in order to weight the amount of plume emissions incorporated into a particular layer. If both  $h_t$  and  $h_b$  are contained within a particular layer, all the plume's emissions are allocated into one layer. As noted above, the number of layers receiving plume emissions is also dependent on the number of vertical layers in the model. A model configuration with fewer vertical layers generally implies greater layer thicknesses.

#### 4.4.5 Generation of 3-D Emissions

Once the plume rise and plume partitioning functions have been performed, the emissions from each point source plume are transferred to the 3-D emission array which also contains the surface area emissions in the first layer. The 3-D emission array is written at an hourly interval for the entire simulation period to a data file in a format compatible for use in CCTM simulations.

### 4.5 Data Requirements

The following items are the data input requirements for operation of MEPPS. Those items that must be supplied by the user are marked (U). Those items that are fixed internal lookup tables, provided with Models-3, or that may be generated in MEPPS are marked (I).

- Complete annual (point, area, and mobile-source data by source category code) Regional, National, or international emission inventories are necessary for regional modeling. The inventories preferably should be in the ASCII format of the EPA National Emission Trends (NET) inventories. However, IDA allows import and conversion of any inventory with known fields formats in ASCII, SAS, or NetCDF format. Currently, the 1985 NAPAP, 1988 National Inventory, 1990 National Interim Inventory, and 1990 National Emission Trends (NET) inventories for criteria pollutants are included. Limited data for southern Canada are available as a part of these inventories (I). Emission inventories for other areas, years, or pollutants must be supplied by the user (U).
- Existing hourly emission data, such as CEM data, may be used directly or substituted for hourly emission data derived by temporal disaggregation from annual emission

inventories. The hourly data may be imported through the File Converter and IDA. The Models-3 system includes 1995 CEM data in the SAS data set format provided by the US EPA Office of Acid Rain (I). Other hourly data must be supplied by the user if desired (U).

- Hourly meteorological data for surface temperature and solar radiation, in NetCDF I/O API format, (from MM5 processed via MCIP) must be available for modeling biogenic or mobile source emission data. If data files for the appropriate case area available, the user may select them in MEPPS or when running Study Planner. Otherwise, it is necessary to first run MM5 and output the meteorology files through MCIP (I).
- Chemical speciation profiles matched to source category codes are necessary for the speciation processor (I). These may be updated with new information.
- Temporal allocation profiles, by source category code, must be available to accomplish temporal allocation of emission data to hourly emission data (I). These may be updated with new information
- Geographic coverages for surrogate spatial allocation (gridding) of emission data. The user may supply additional coverages: Those supplied with MEPPS include (I):
  - Political boundaries at the county level for North America
  - Land-water boundaries and features for North America
  - County-level population information for North America (with a gridded surrogate for Canada)
  - Federal Highway Administration major highway coverage for the United States
  - TIGER-LINE detail road coverage for the United States
  - Land cover for North America. Currently is at county-scale for the United States and gridded at coarser resolution for Canada and Mexico.
  - Land cover for the United States at one kilometer resolution is anticipated in 1999
- Species emission factors for biogenic emission modeling (I)
- Standard Mobile 5a model input information by political area (usually state and/or county), including vehicle fleet composition data, fuel type use by geographic area, inspection and maintenance program information, etc, (U). A template with examples is provided for the user to edit.

- Road silt loading, geographic distribution of paved and unpaved roads, vehicle fleet composition data, fuel use data, and inspection and maintenance data are necessary as input to the PART5 mobile particulate model.
- Geographic, source category code-specific growth projection factors. These are provided for use with MEPRO (I).
- Source category and/or geographically specific emission control data, and regulatory factors including control efficiency, rule effectiveness, and rule penetration for use in MEPRO. These must be supplied by the user because controls are not standard, and in fact are a key variable in examining different emission scenarios (U).

#### **4.6 Plans for Improvement**

Plans for improvement of MEPPS may be divided into long and short-term improvements. The short-term improvements are those that are anticipated to be in the Models-3 release scheduled for the summer of 1999.

##### **Short-term Improvements**

- The IDA will be improved to consolidate and further automate much of the quality control processing, format and unit conversion, and data file manipulation. In particular, format templates of internal formats will be added to assist importing of emission data files into the system, and quality control for the CEM data will be enhanced.
- Although SAS<sup>®</sup> has proved to be a useful tool to date, increasing data handling requirements will likely overwhelm the data handling capabilities of SAS<sup>®</sup>. Therefore, it is necessary to convert MEPPS to a fully Models-3 framework compliant system in order to take full advantage of the or object-oriented data base architecture of the system (eg., Orbix<sup>®</sup>) to more efficiently manage very large amounts of data. The use of the Sparse Matrix Operator Kernel Emission (SMOKE) system, in conjunction with the Models-3 object-oriented architecture and expansion of existing functionality should substantially improve performance because relatively inefficient processing sequences will not be necessary, and it will not be necessary to manipulate all elements of large files for each operation. More information about SMOKE can be found in Coats et al. (1995). An initial (but not complete) version of SMOKE is planned for installation by summer 1999.

##### **Long-term Improvements**

- New mobile source emission estimation models are being developed by the U.S. EPA Office of Mobile Sources. They are scheduled for completion late summer of 1999. Mobile 6 will replace Mobile 5a and Mobile 5b, and an Off-road Mobile Source Model

will be introduced. These models will be installed in MEPPS when they are available and resources allow.

- The MEPPS contains the split factor assignments for two common chemical speciation mechanisms, CB-4 and RADM 2, that may be selected by users. These speciation mechanisms will also be in SMOKE. There are plans to also install the split factor information and computational mechanisms necessary to use for the Statewide Air Pollution Research Center (SAPRC) (Carter, 1988), and eventually, code necessary to support the more complex Morphecule mechanism being developed at the University of North Carolina.
- Additional quality control and reporting capabilities will be added to SMOKE, equaling or surpassing those capabilities in currently in MEPPS.
- The emission data processing system could be enhanced to support nested grid structures. Currently, there is only limited support for nested grid structures and no support for multiscale grid structures. Under the current formulation, EMPRO (including the gridding processor) must be run consecutively for each grid structure that exists within the nested grid structure. Repetitive runs are inefficient, and computer resources are poorly utilized because certain areas in the modeling domain will be processed more than once. In addition, the gridding processor cannot generate rotated grids, which may be a limitation for some applications. If an air quality modeling study requires a rotated emission modeling grid, a knowledgeable ARC/INFO<sup>®</sup> user must prepare the grid independently from menu options provided in Model-3 and MEPPS.
- Tools such as NetCDF and the I/O API will evolve to directly accommodate geographic data references in their structure. This will allow manipulation of geographic data (gridding, for example) to be accomplished without the use of non-conforming commercial software tools now in Models-3 system.

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